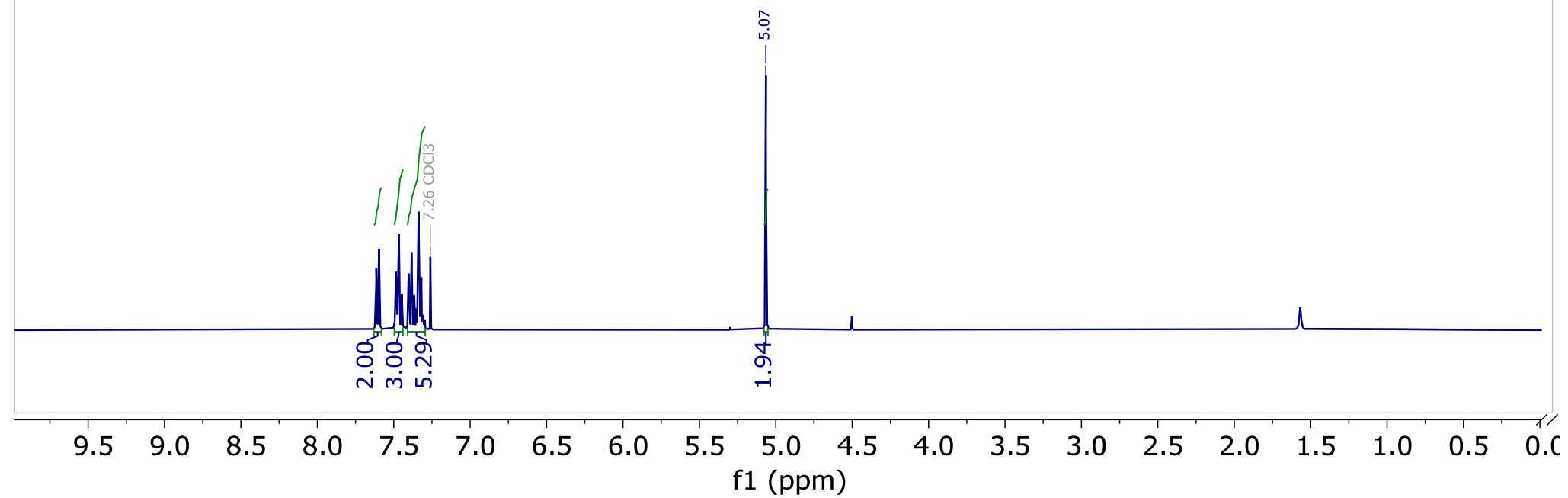
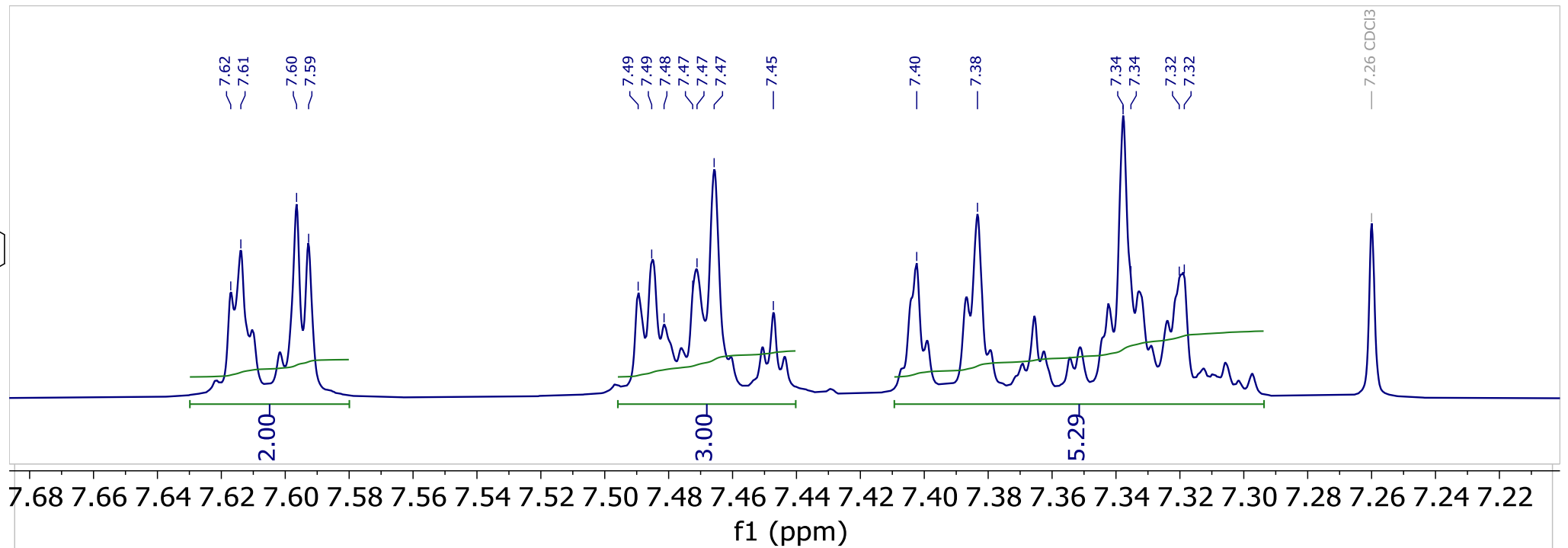
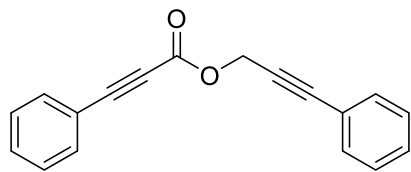


**Supplementary Material for Case Study # 1**  
**The Hare and the Tortoise: Slow and Steady Gets You the Correct Target!**

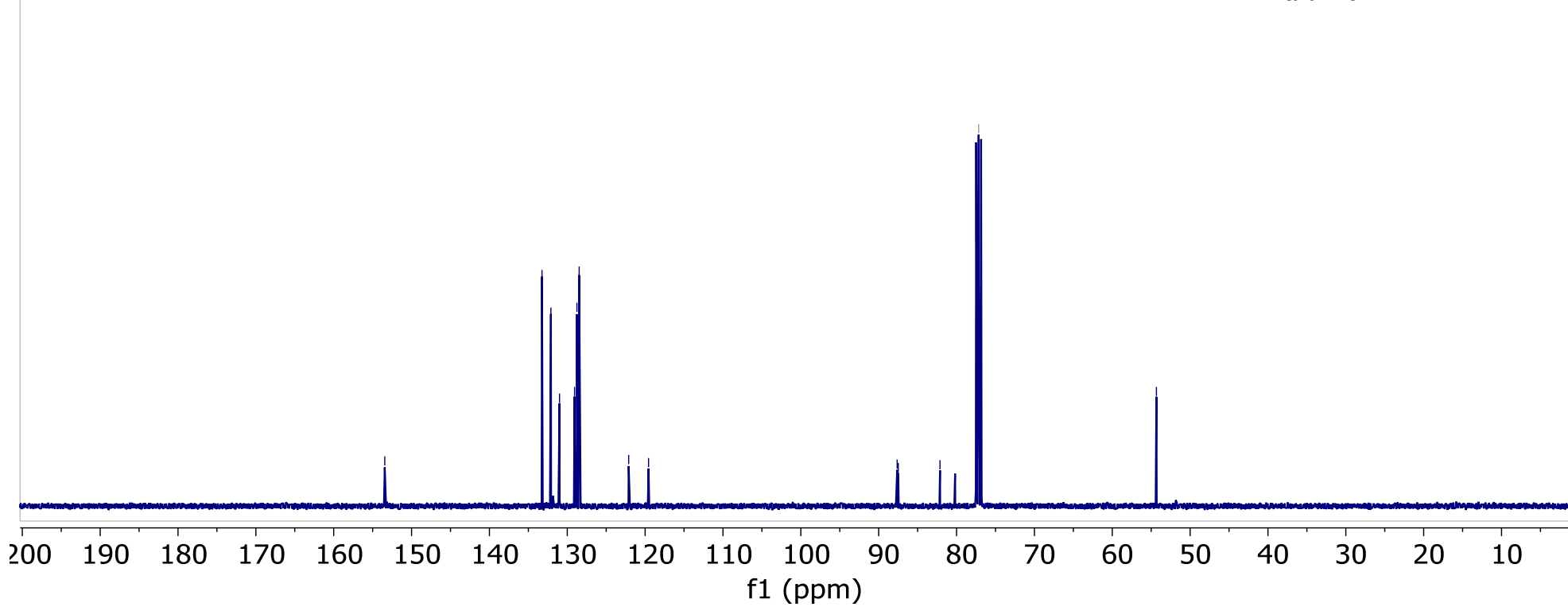
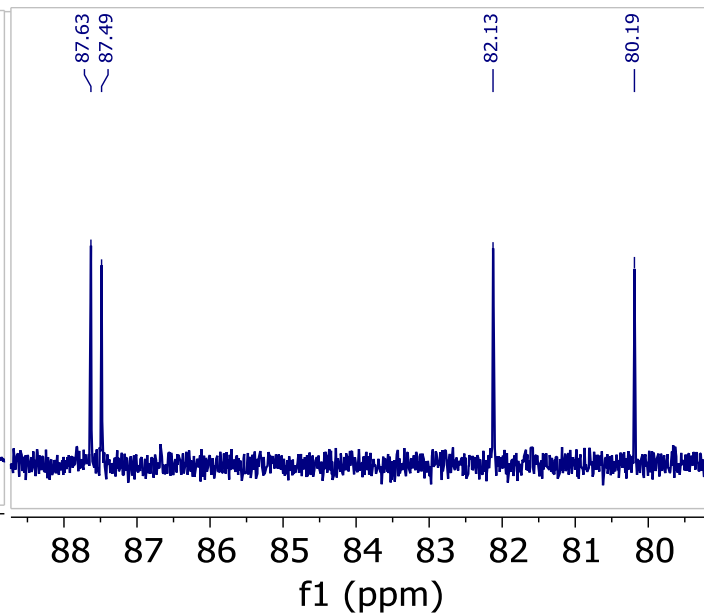
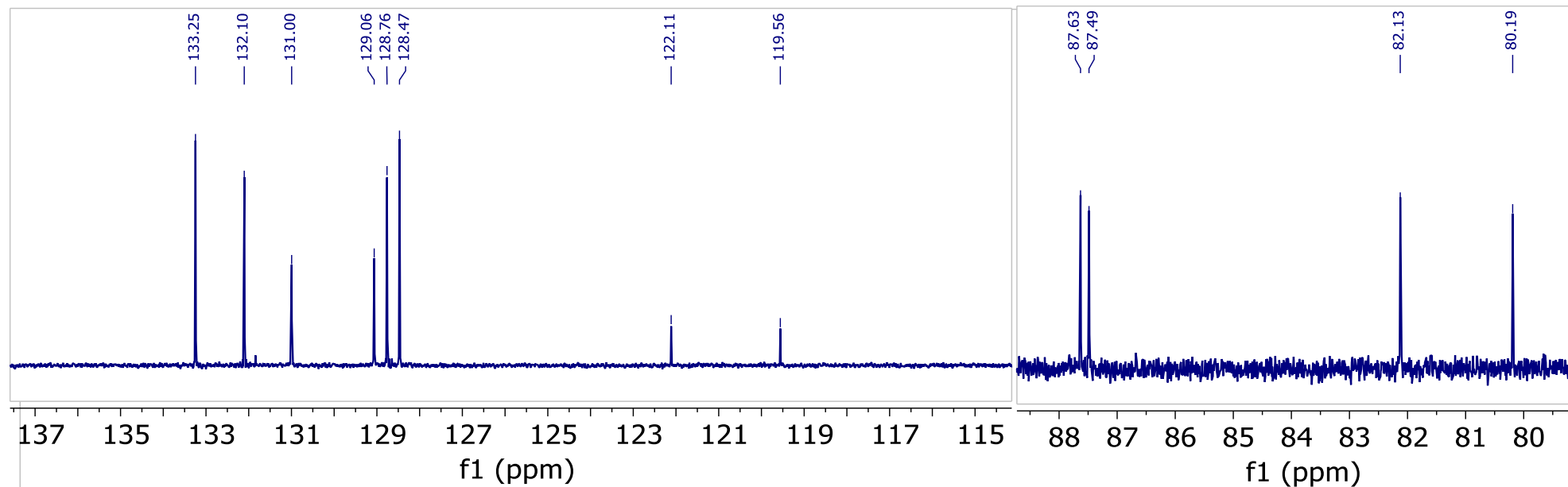
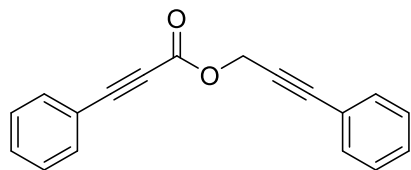
FIGURE	DESCRIPTION	PAGE
S1	Ester 1 - $^1\text{H}$ NMR	S1
S2	Ester 1 - $^{13}\text{C}$ NMR	S2
S3	Ester 1 - IR	S3
S4	Compound 1 - $^1\text{H}$ NMR	S4
S5	Compound 1 - $^{13}\text{C}$ NMR	S5
S6	Compound 1 - APT	S6
S7	Compound 1 - COSY	S7
S8	Compound 1 - COSY (Zoom)	S8
S9	Compound 1 - HSQC	S9
S10	Compound 1 - HSQC (Zoom)	S10
S11	Compound 1 - HMBC	S11
S12	Compound 1 - HMBC (Zoom)	S12
S13	Compound 1 - 1D NOE	S13
S14	Compound 1 - IR	S14

FIGURE	DESCRIPTION	PAGE
S15	Compound 1 - Mass Spectrum	S15
S16	Compound 2 - $^1\text{H}$ NMR	S16
S17	Compound 2 - $^{13}\text{C}$ NMR	S17
S18	Compound 2 - APT	S18
S19	Compound 2 - COSY	S19
S20	Compound 2 - COSY (Zoom)	S20
S21	Compound 2 - HSQC	S21
S22	Compound 2 - HSQC (Zoom)	S22
S23	Compound 2 - HMBC	S23
S24	Compound 2 - HMBC (Zoom)	S24
S25	Compound 2 - HMBC (Zoom)	S25
S26	Compound 2 - 1D NOE	S26
S27	Compound 2 - IR	S27
S28	Compound 2 - Mass Spectrum	S28

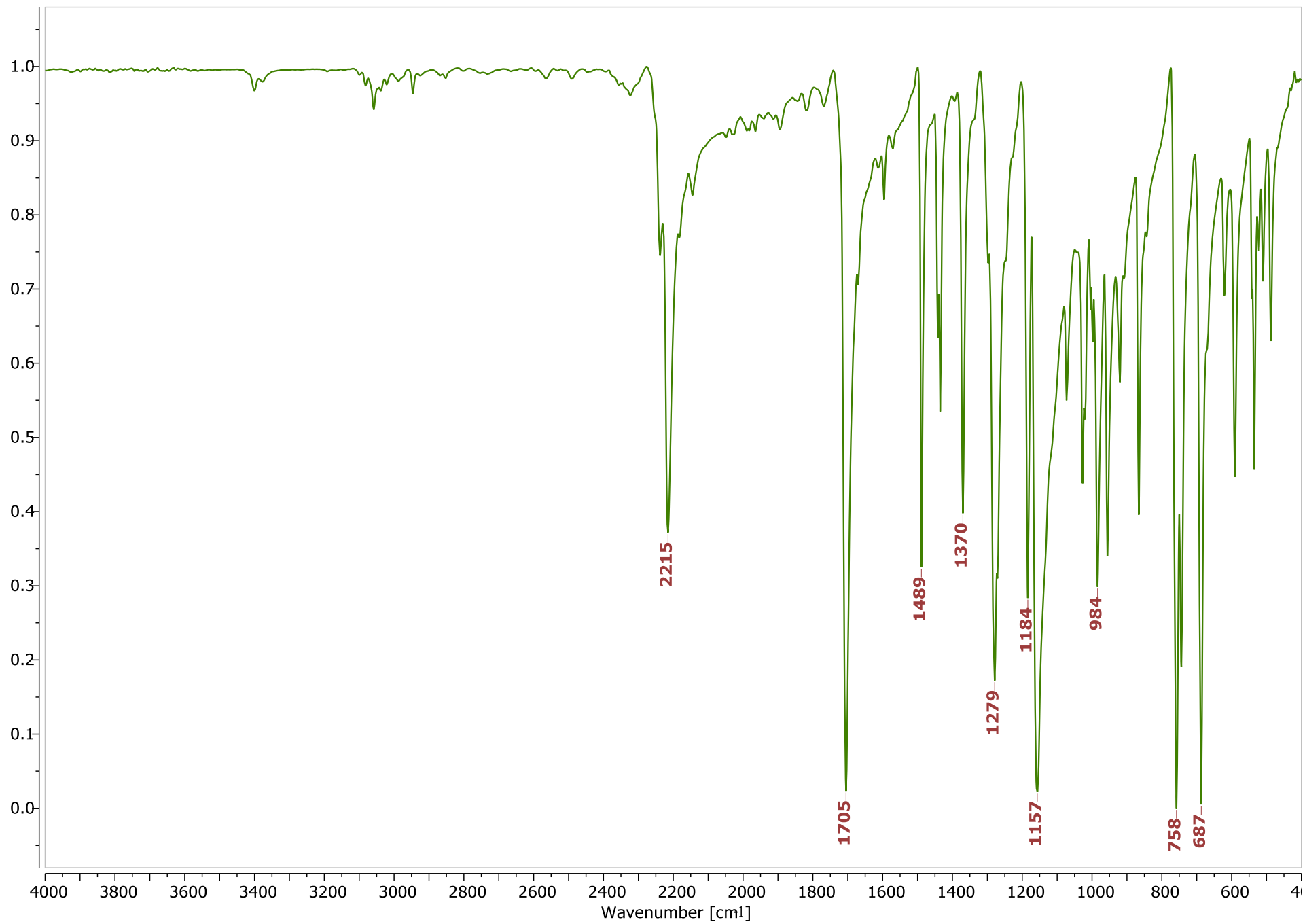
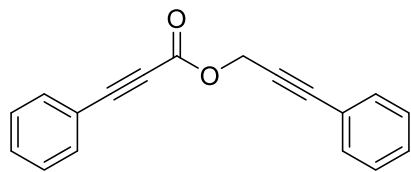
# Ester – <sup>1</sup>H-NMR Spectrum



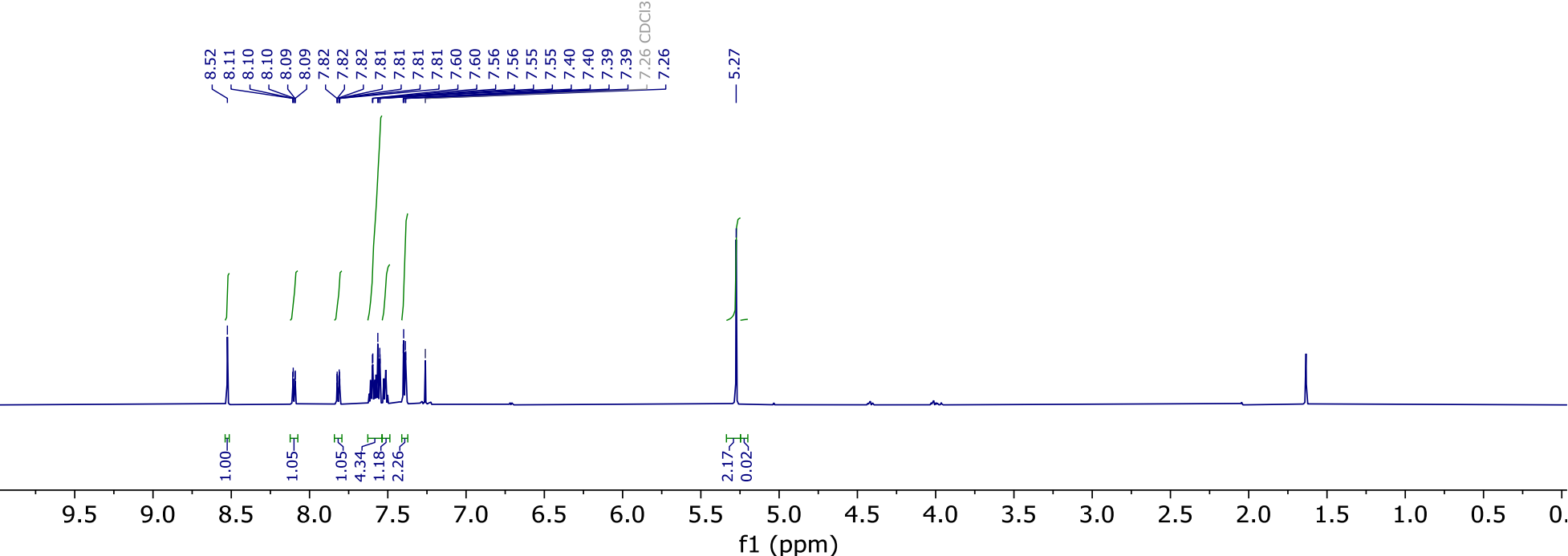
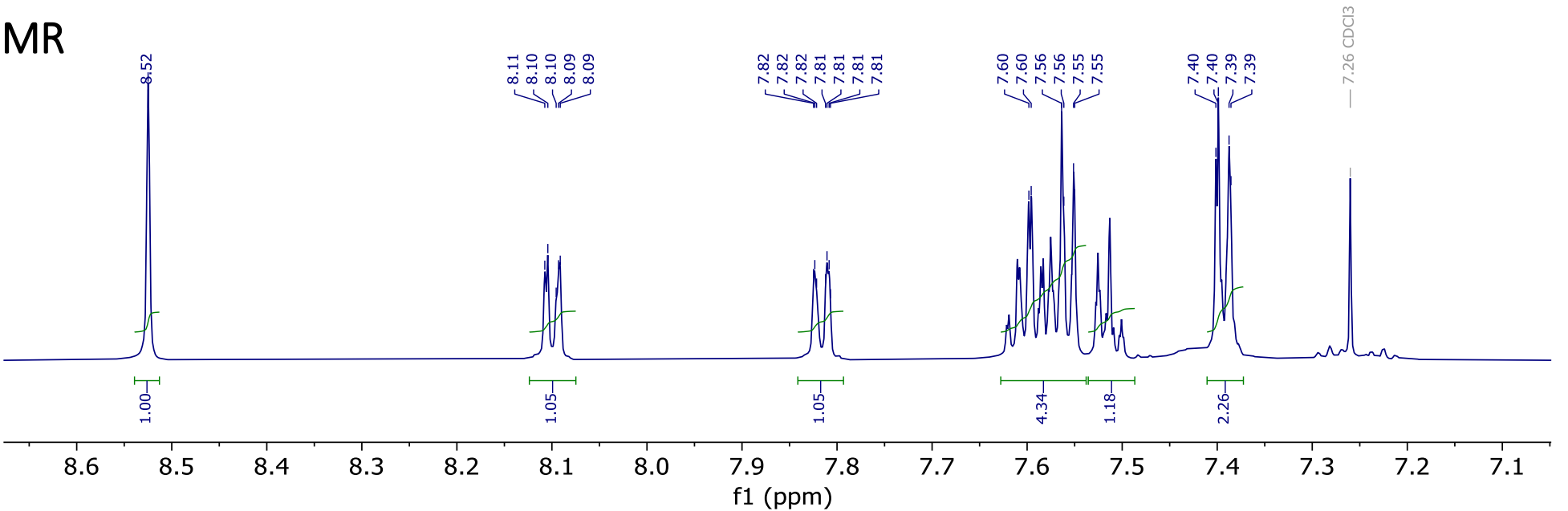
# Ester – $^{13}\text{C}$ -NMR Spectrum



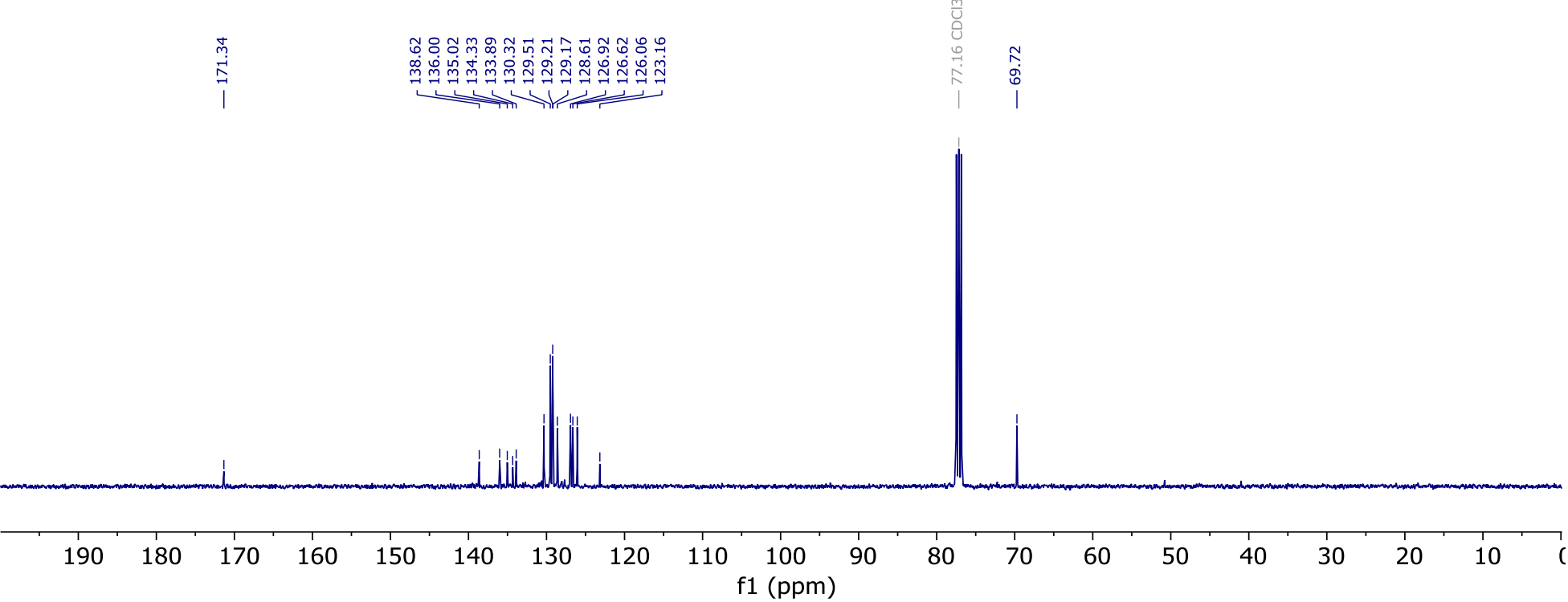
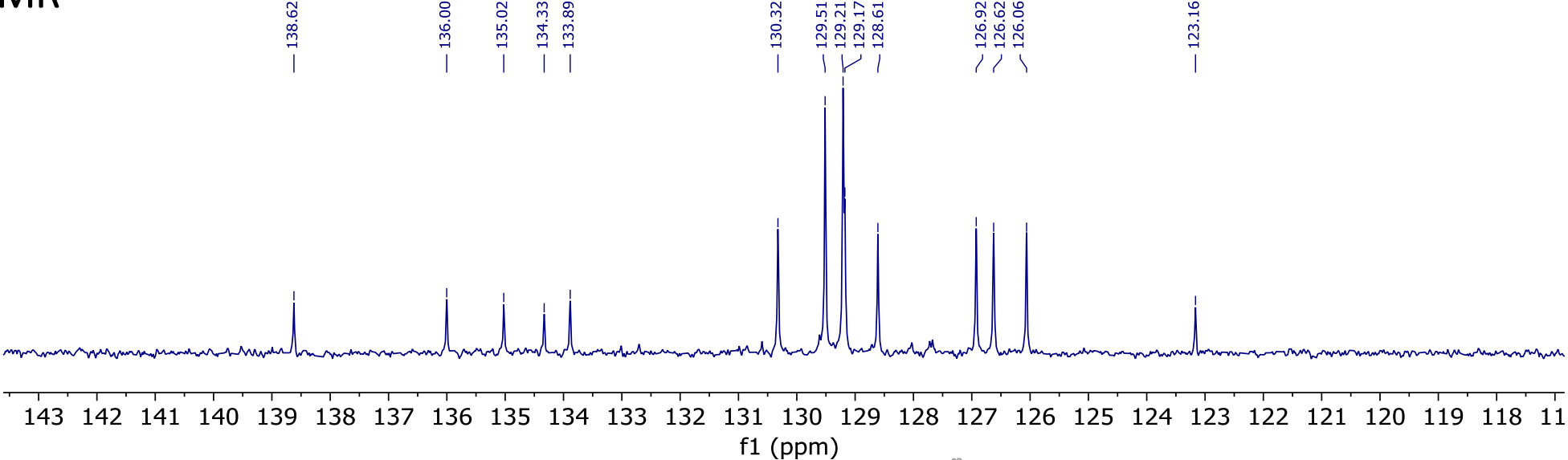
# Ester – IR Spectrum



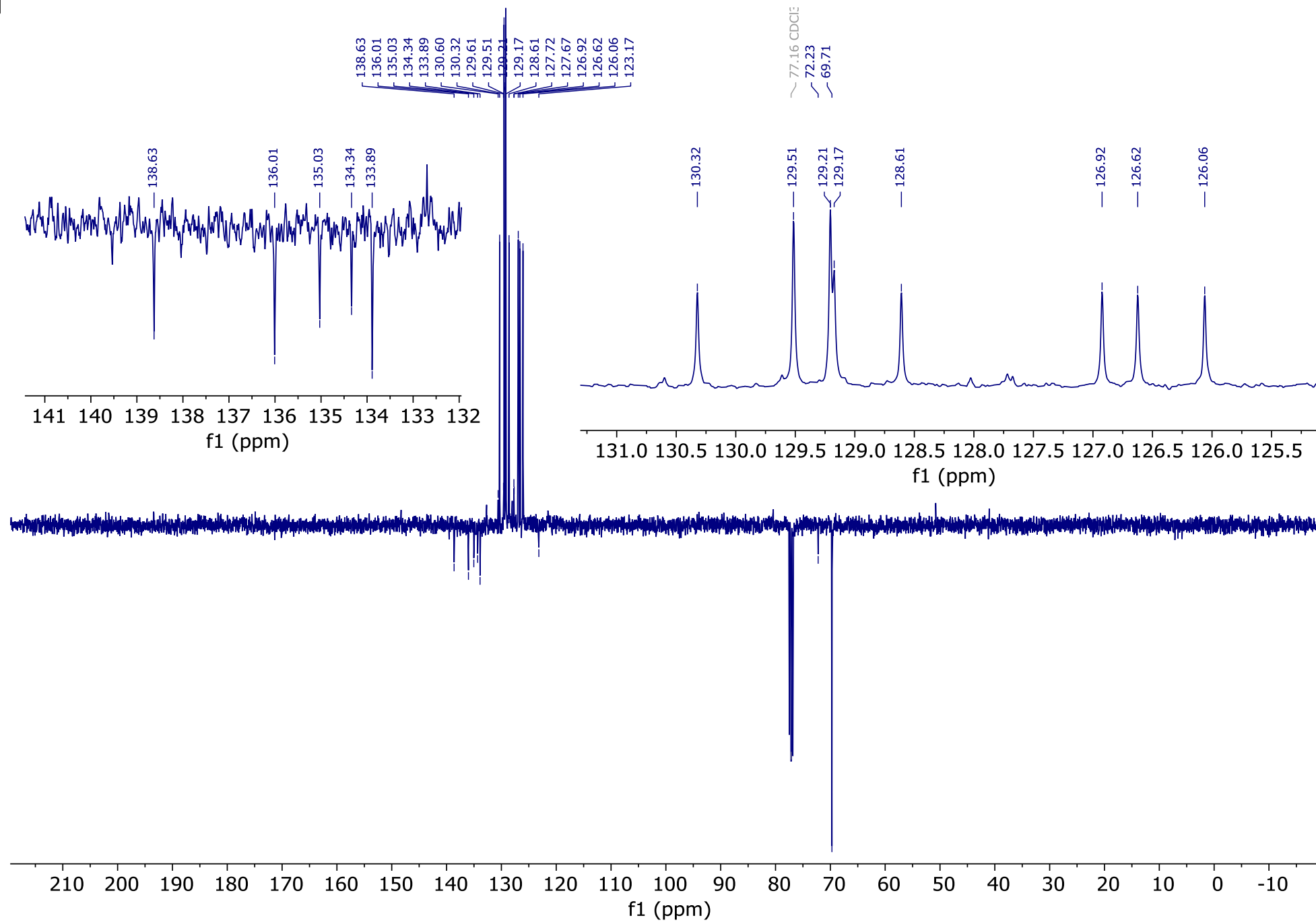
# Compound 1 – <sup>1</sup>H-NMR Spectrum



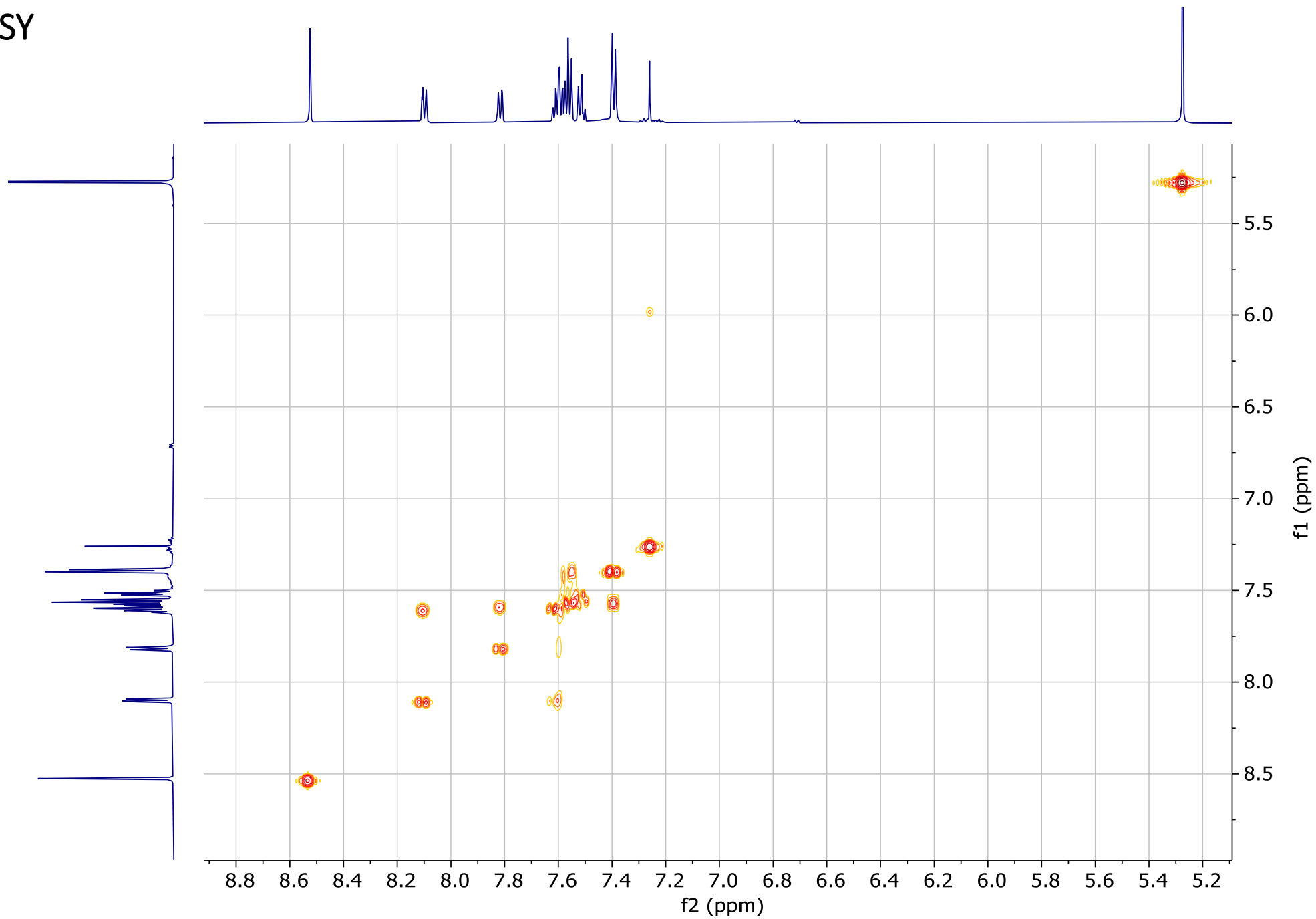
# Compound 1 – <sup>13</sup>C-NMR Spectrum



# Compound 1 – APT Spectrum

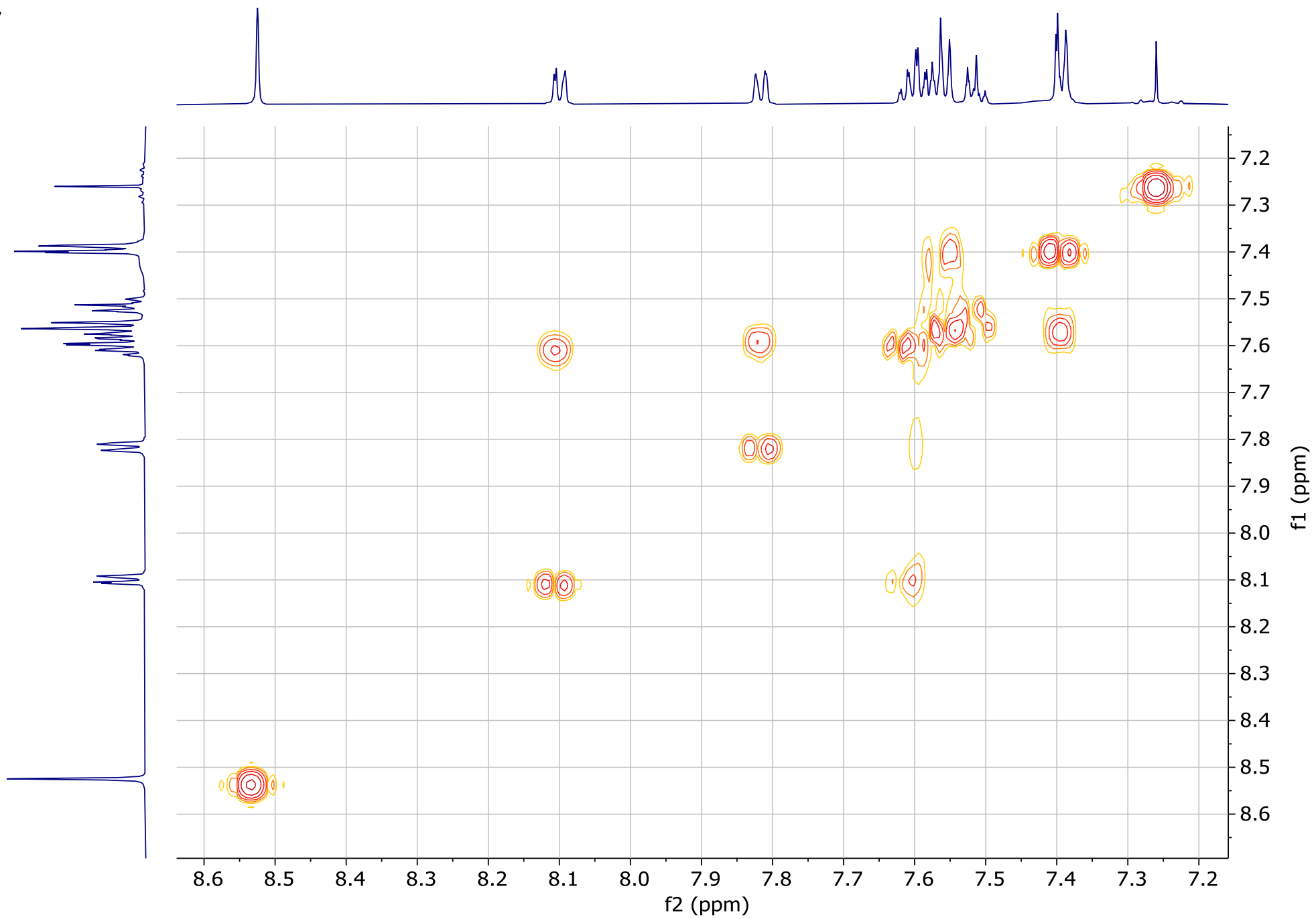


Compound 1 – COSY  
Spectrum

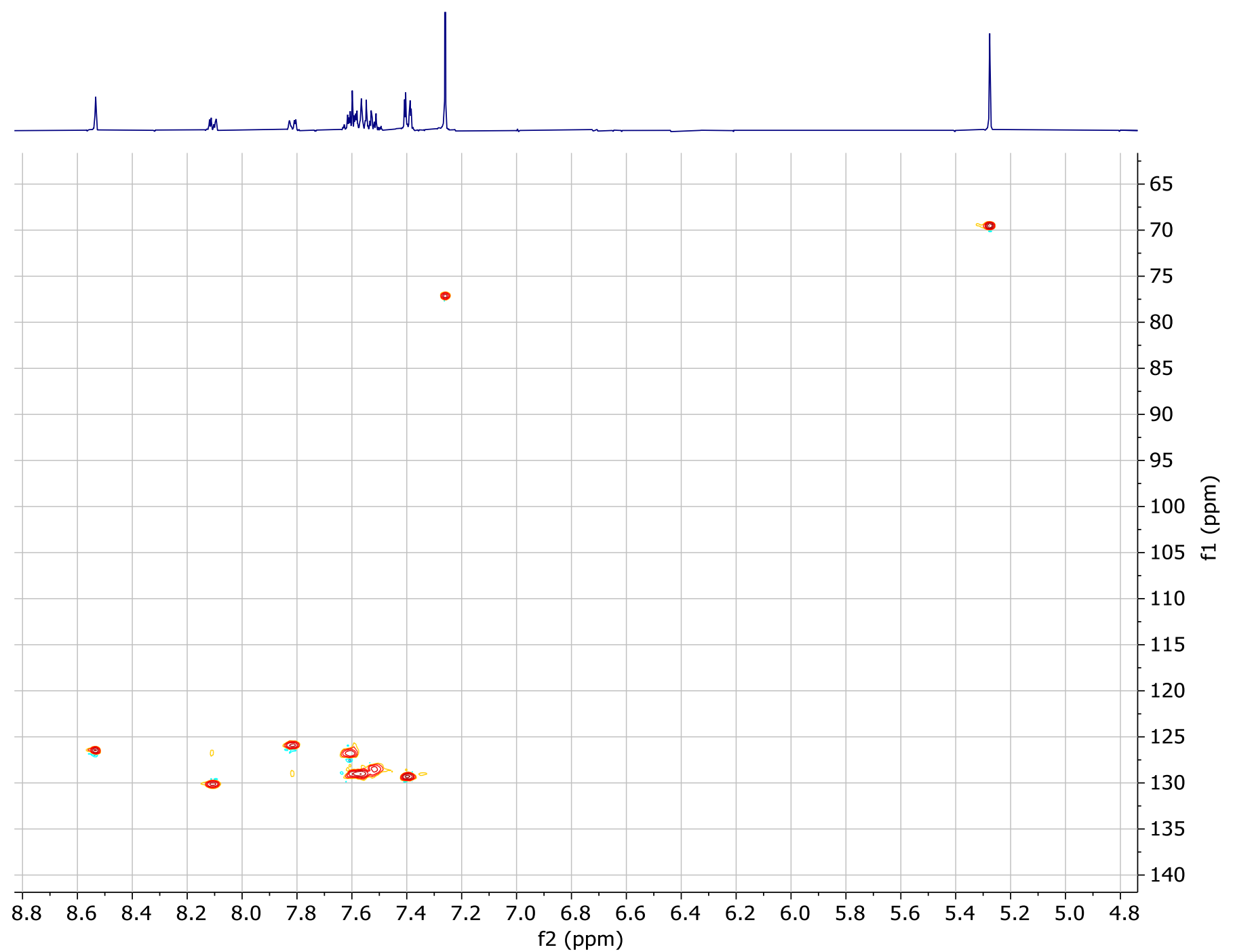




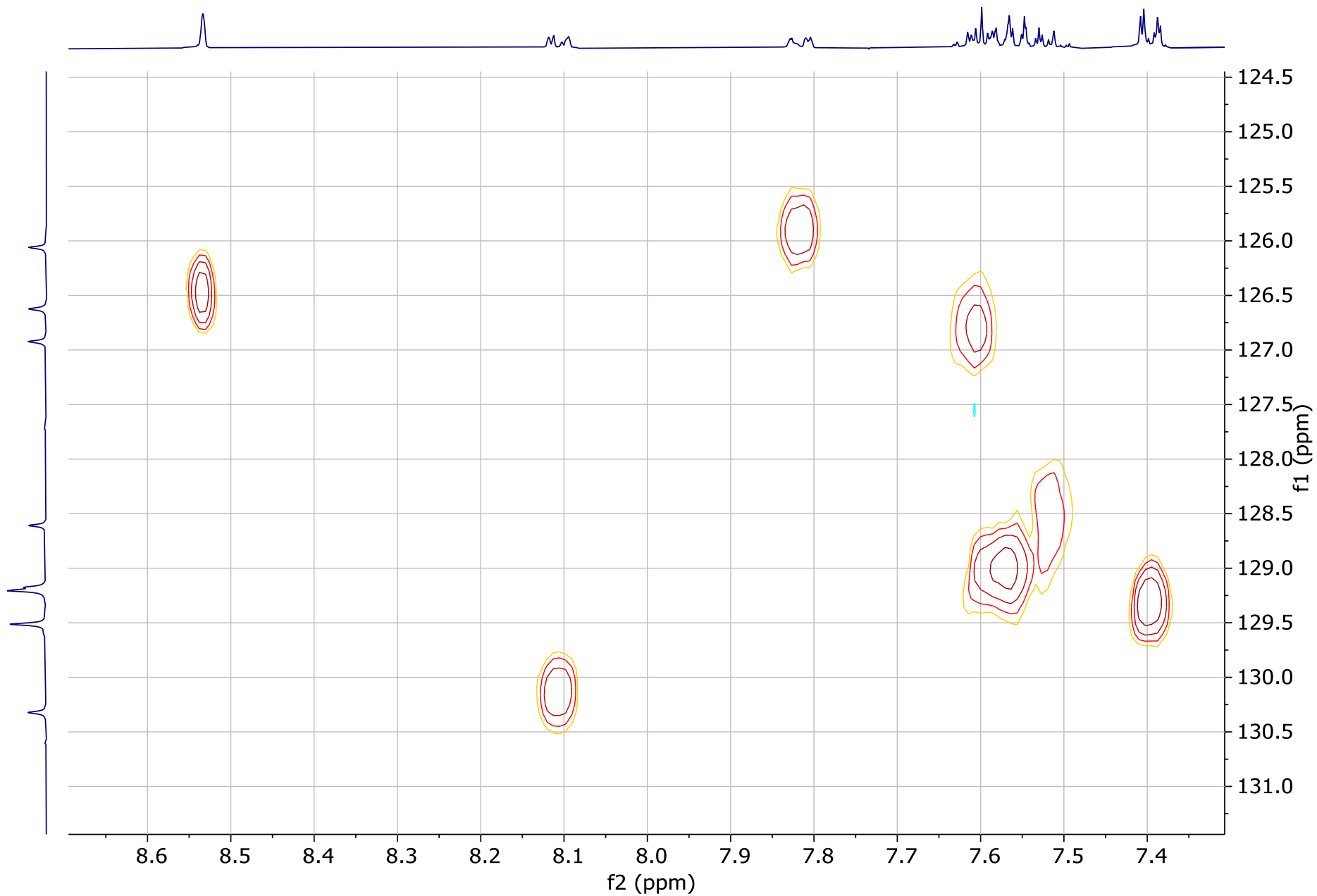
Compound 1 – COSY  
Spectrum (Zoom)



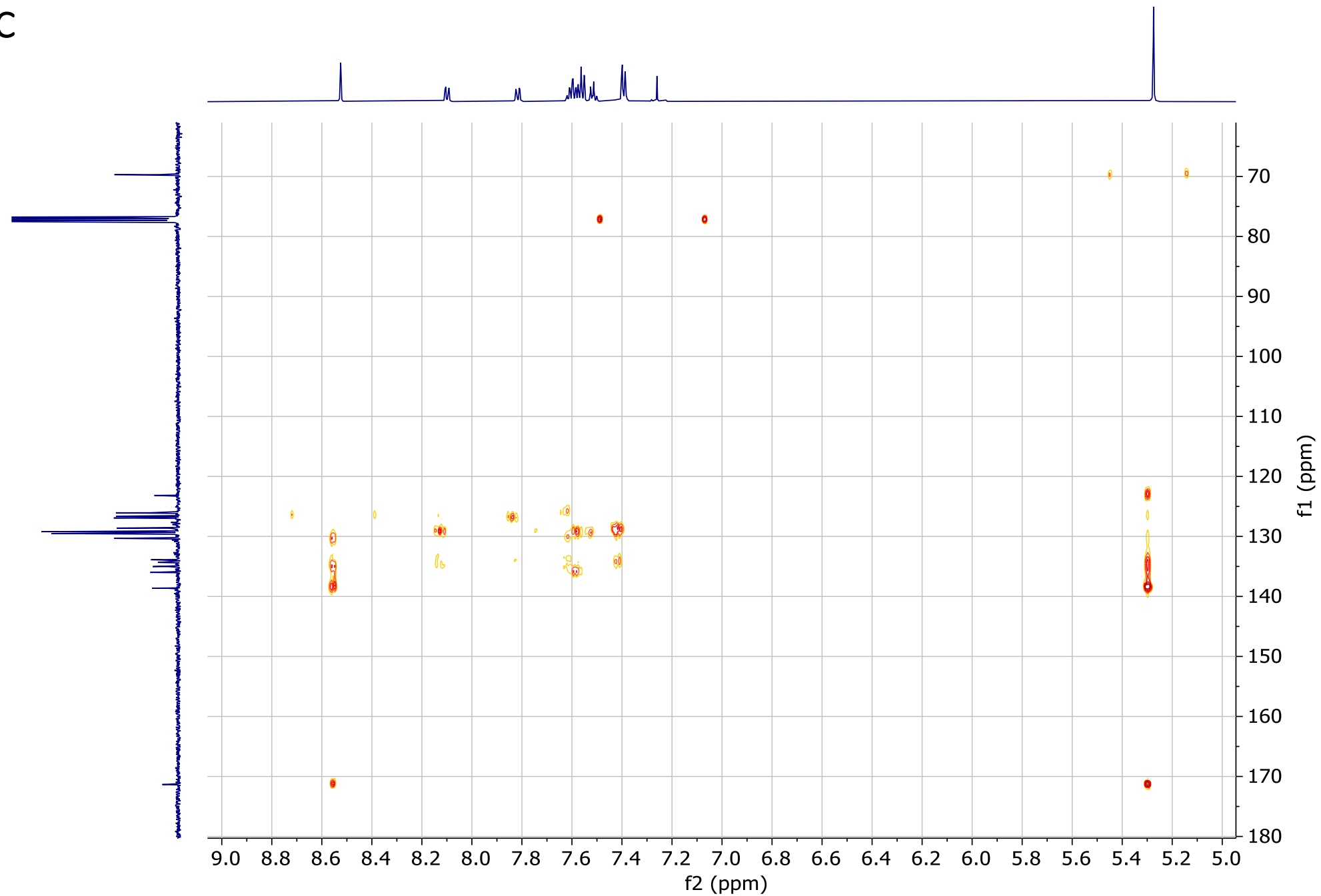
# Compound 1 – HSQC Spectrum



# Compound 1 – HSQC Spectrum (Zoom)

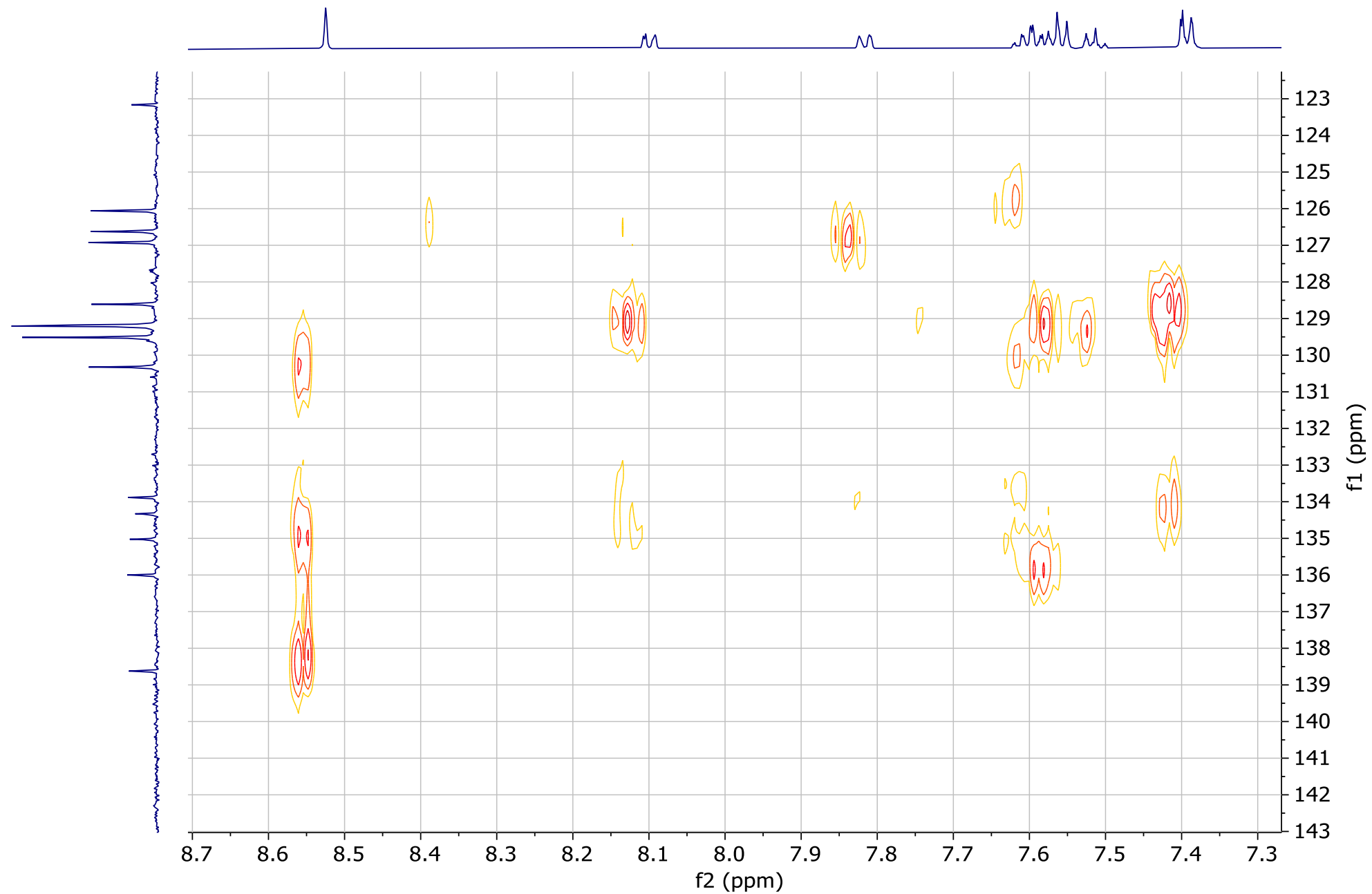


# Compound 1 – HMBC Spectrum

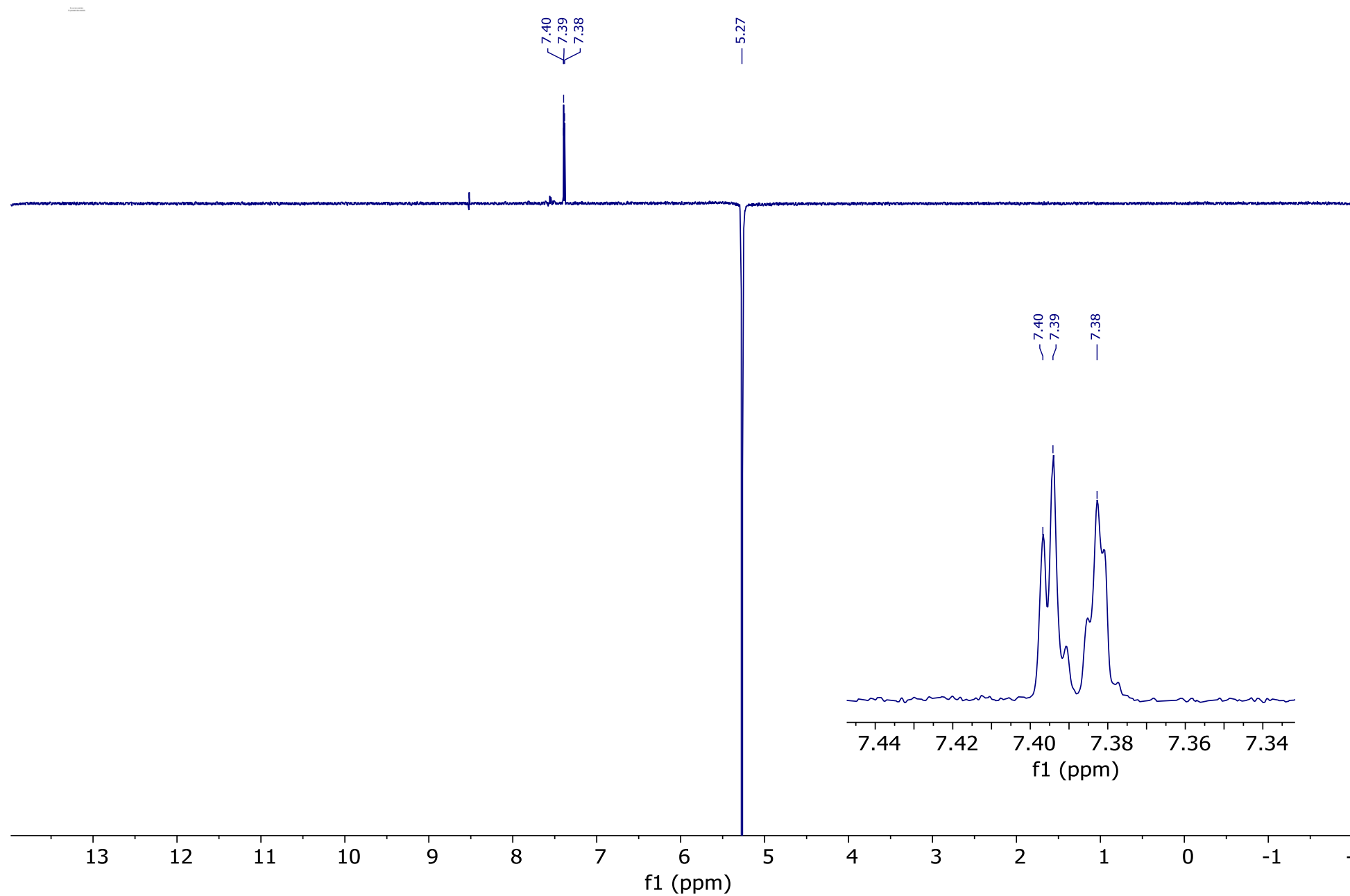


S11

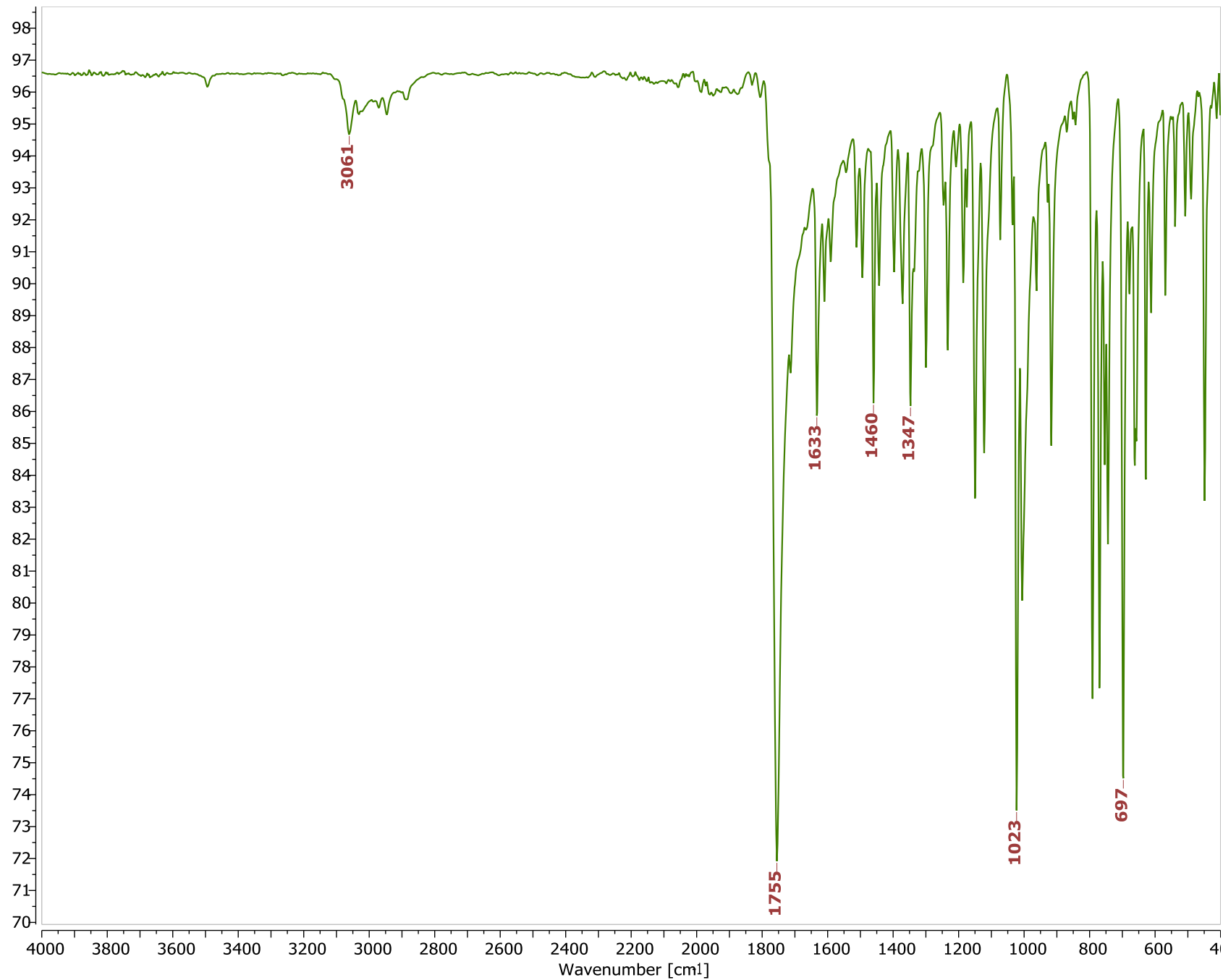
Compound 1 – HMBC  
Spectrum (Zoom)



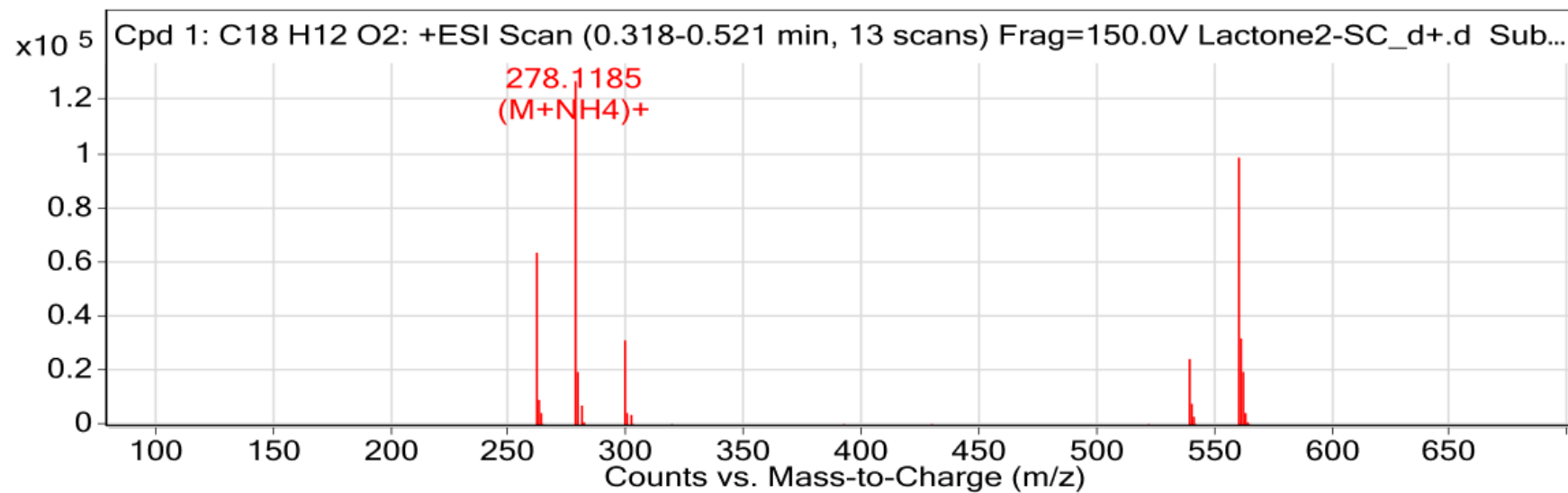
# Compound 1 – 1D NOE Spectrum



# Compound 1 – IR Spectrum



# Compound 1 – Mass Spectrum

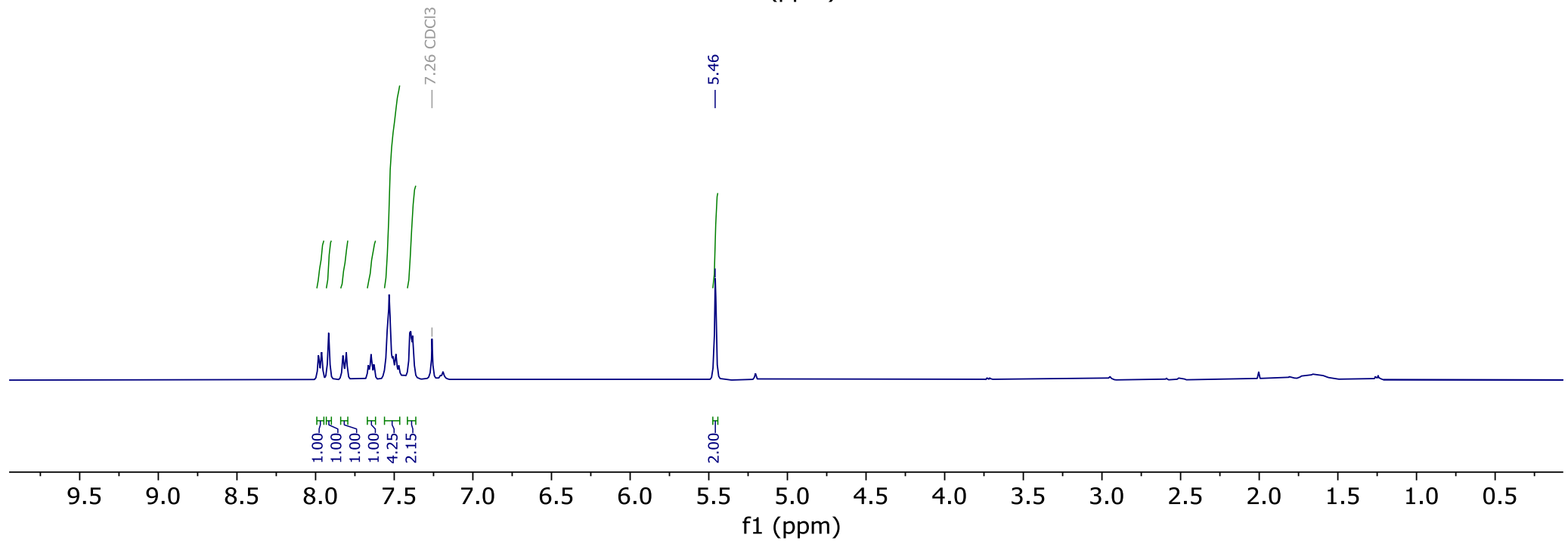
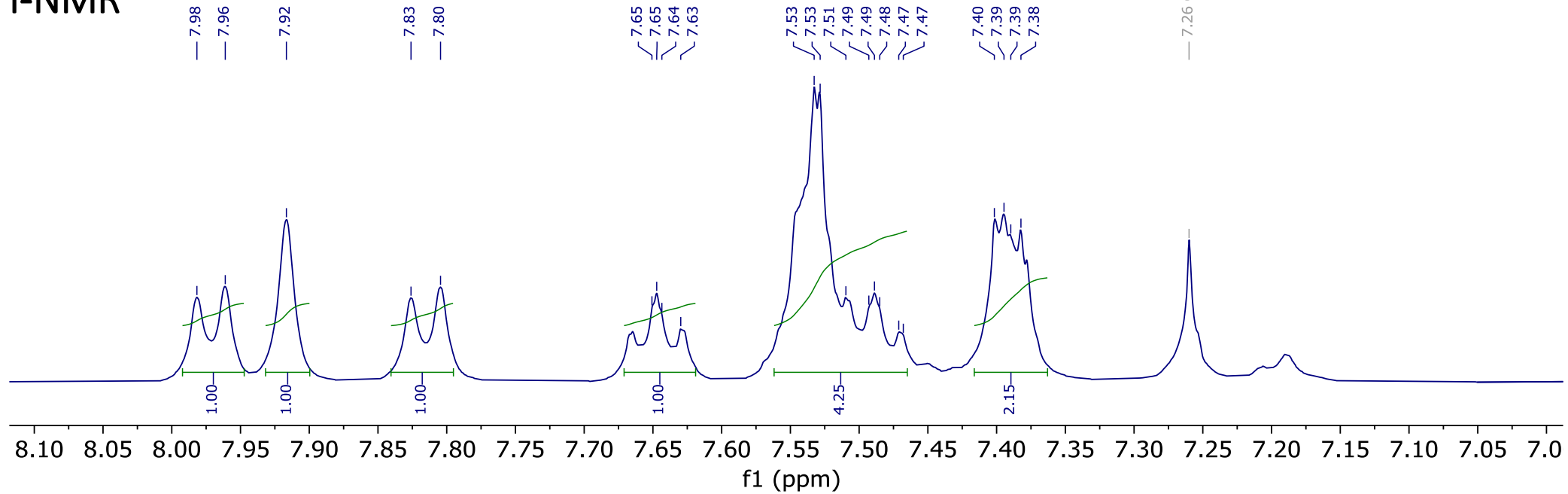


## Peak List

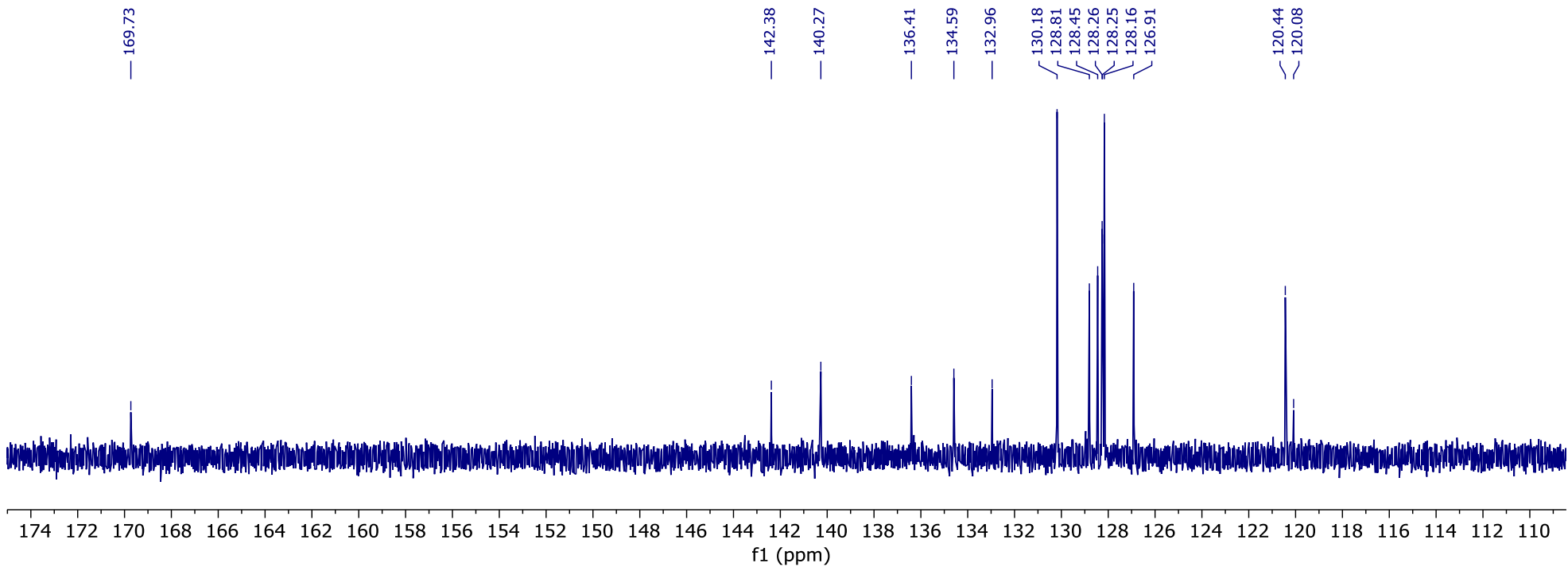
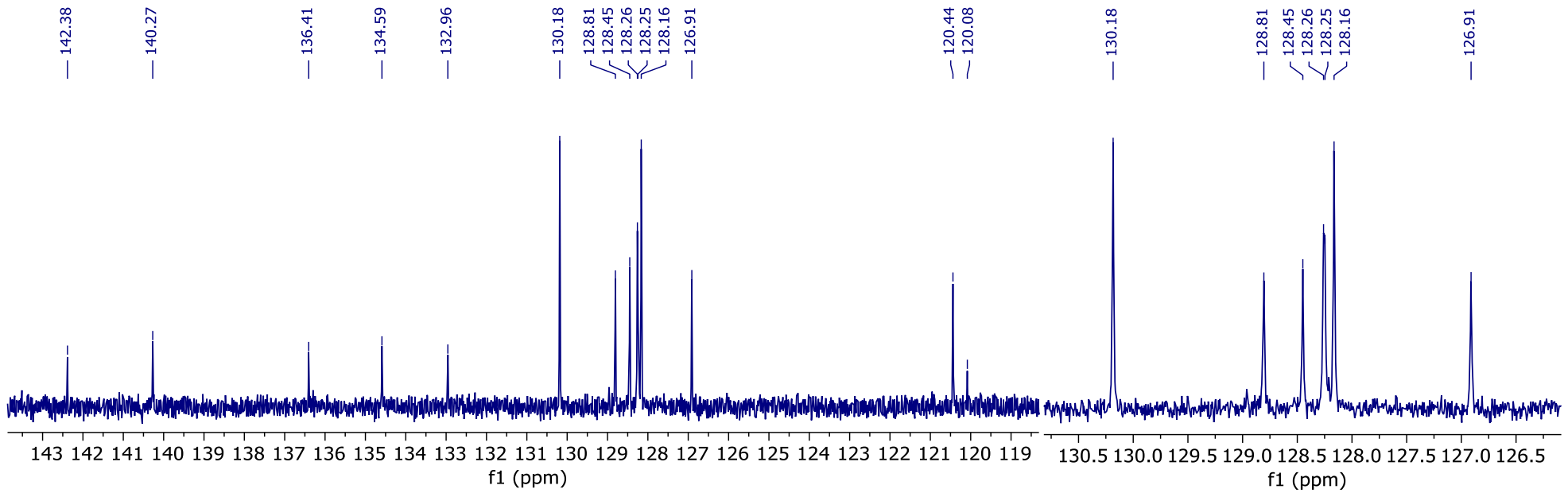
<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
261.0918	1	63705	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
262.0953	1	9659	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
263.1059	1	5072	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
278.1185		127013	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
278.3225		2508		
279.122		19934	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
280.1321		7268	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
299.0481	1	31745	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>
300.051	1	4875	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>
301.0546	1	3806	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>



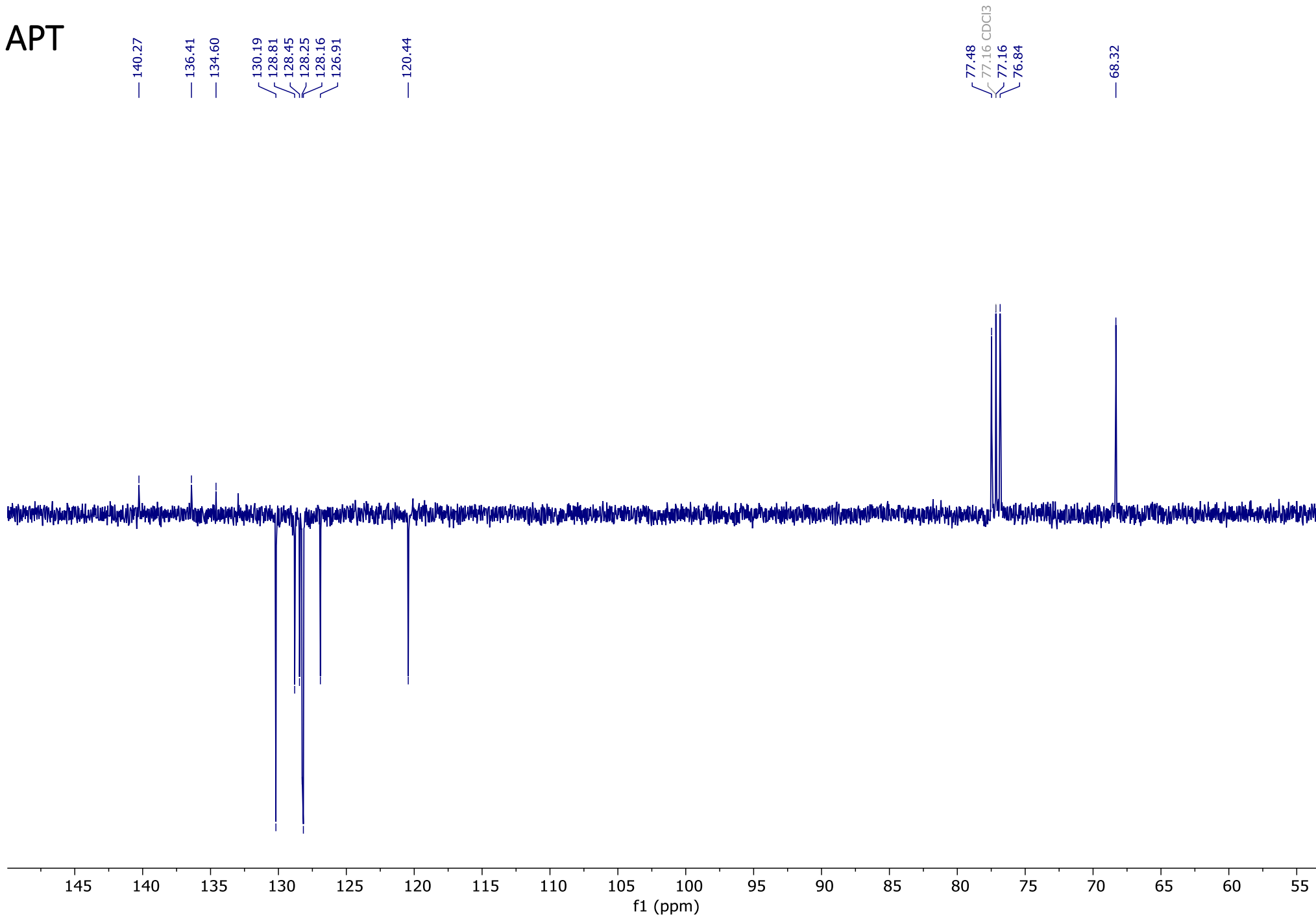
# Compound 2 – <sup>1</sup>H-NMR Spectrum



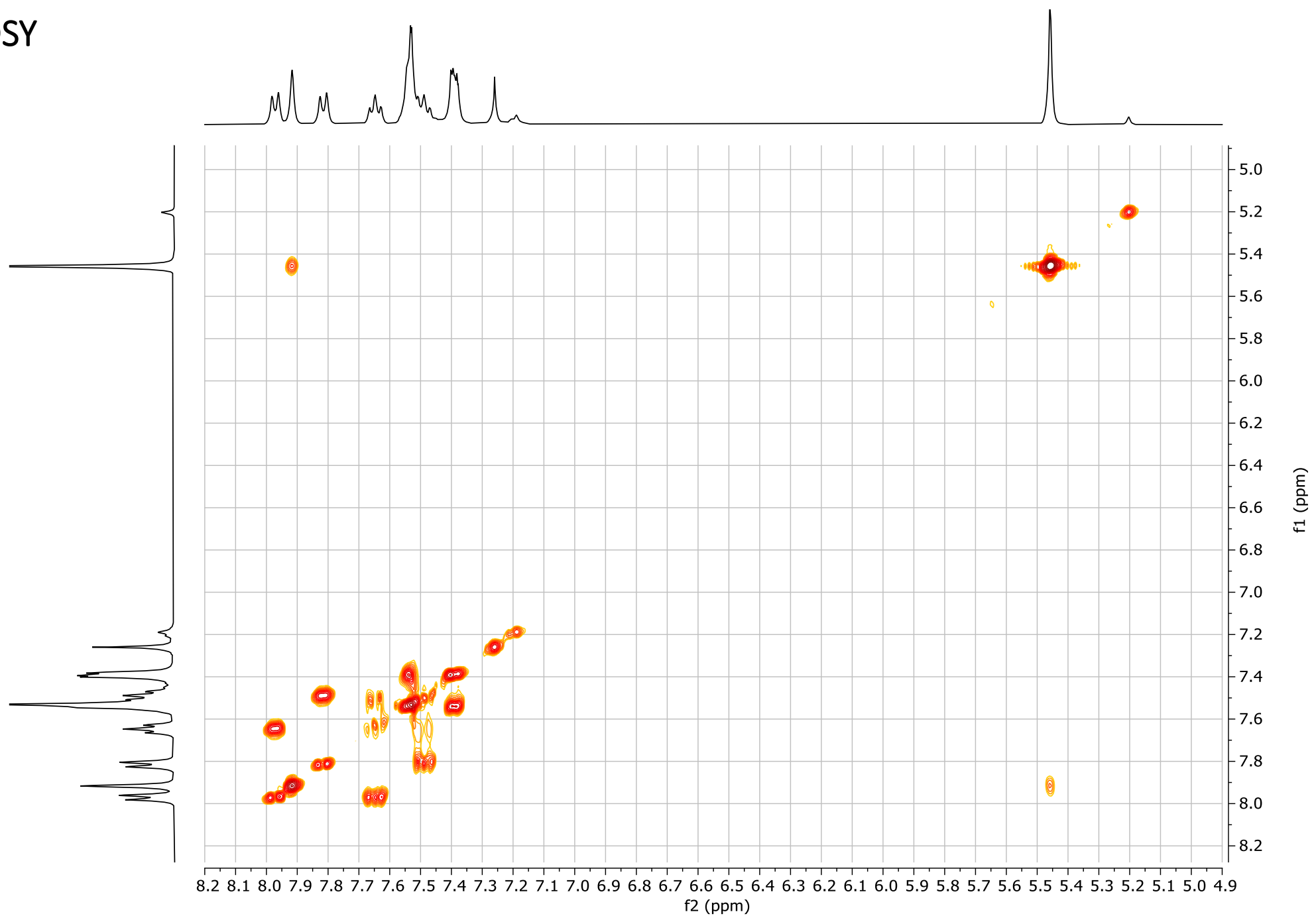
# Compound 2 – <sup>13</sup>C-NMR Spectrum



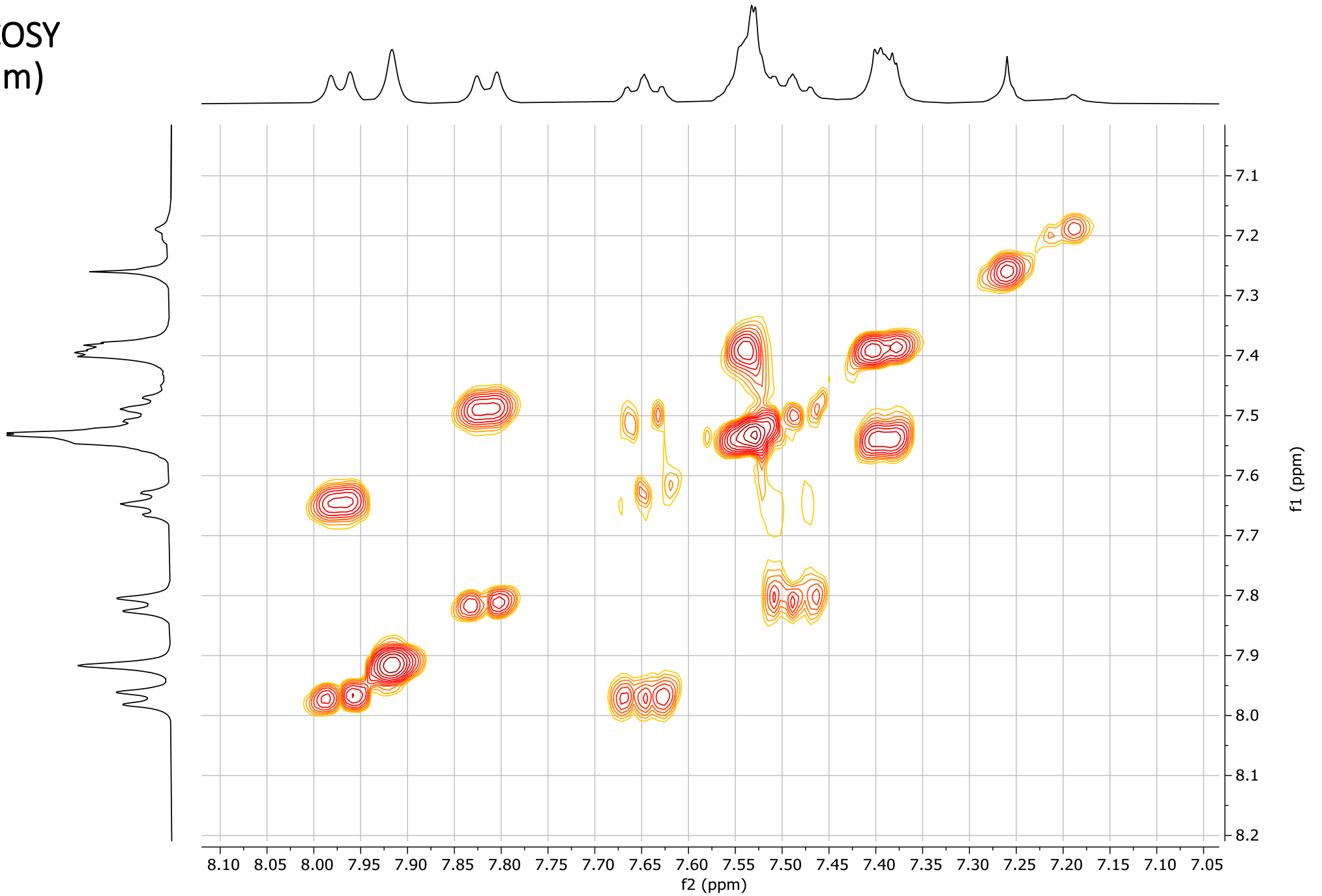
# Compound 2 – APT Spectrum



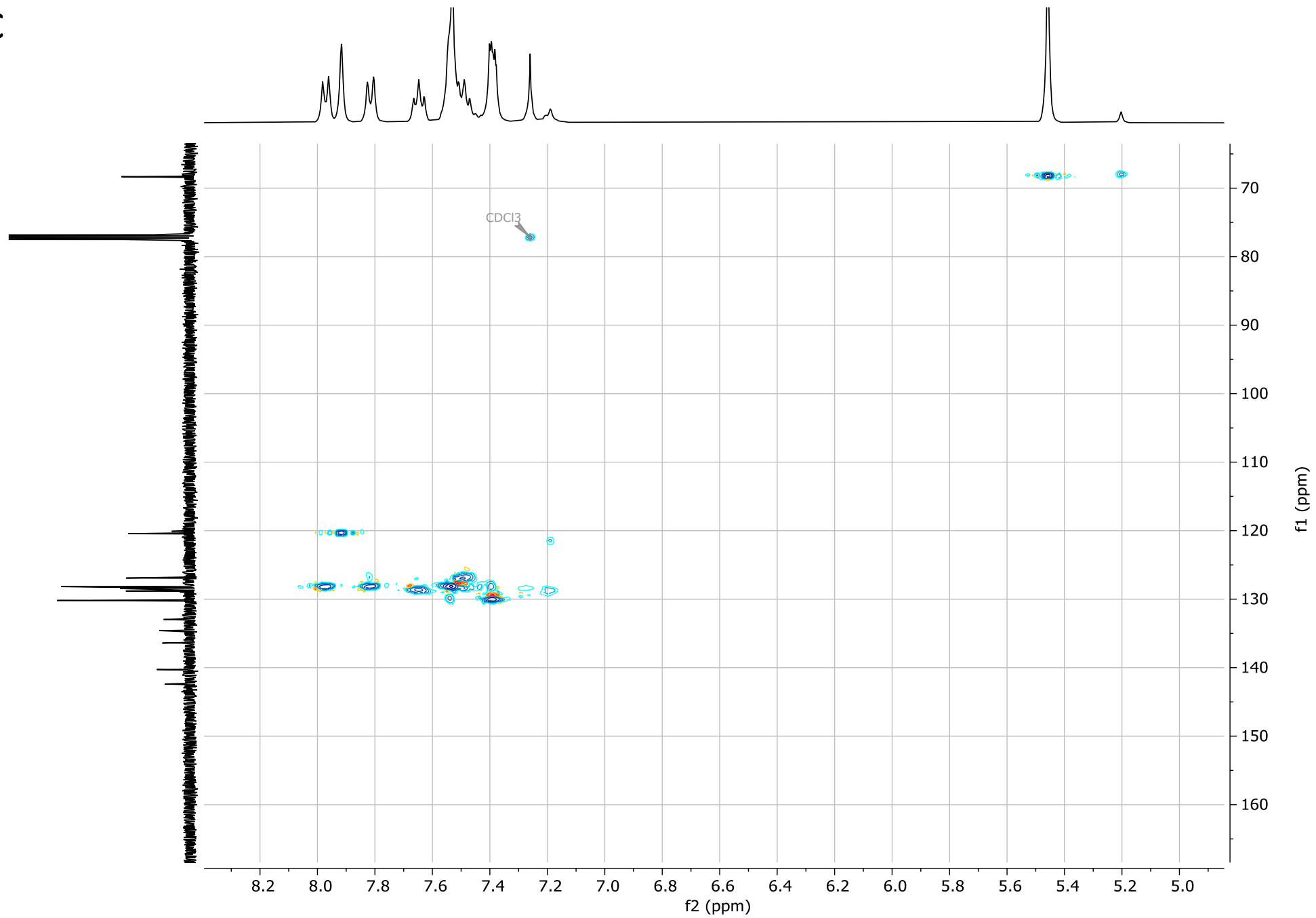
# Compound 2 – COSY Spectrum



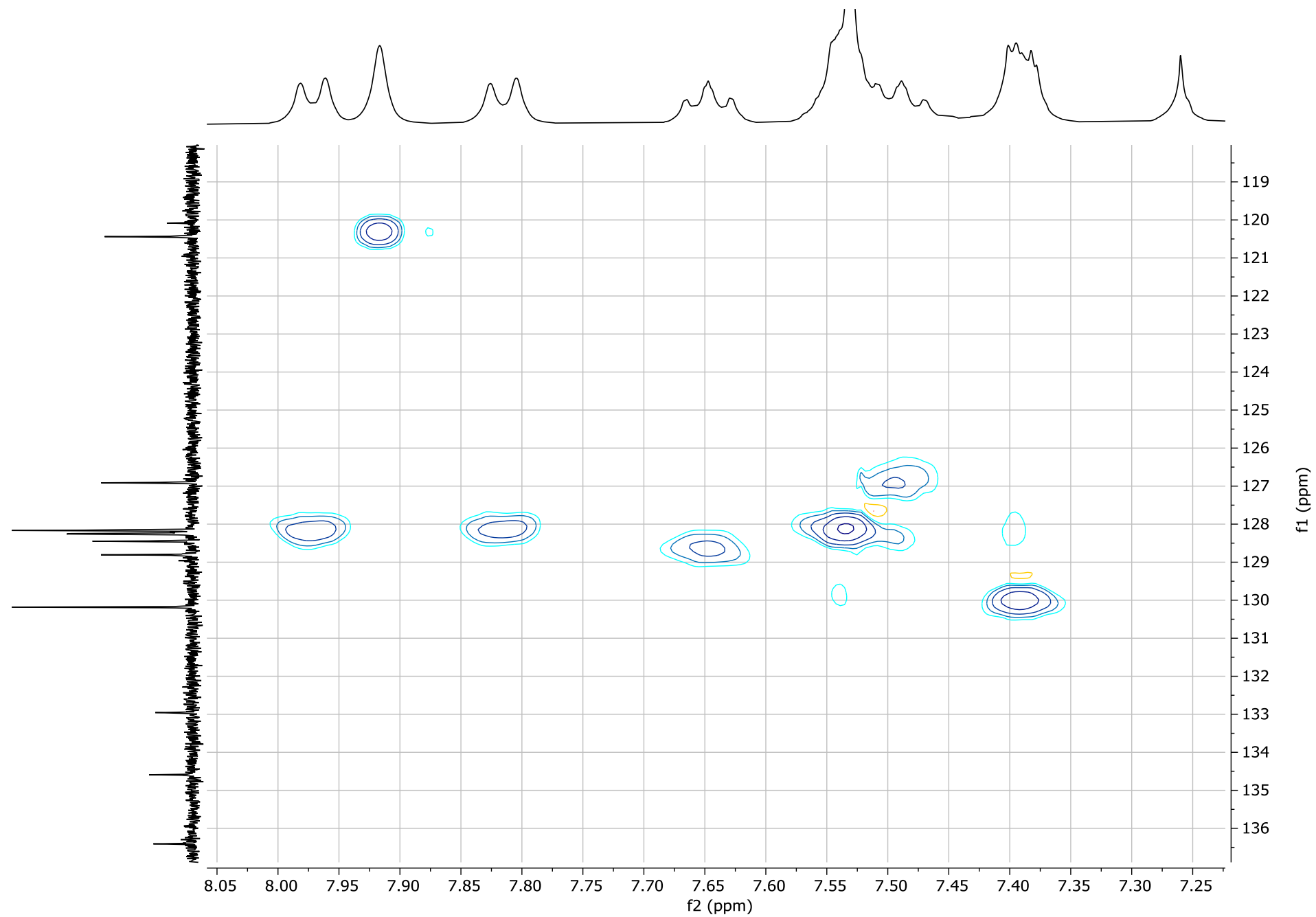
Compound 2 – COSY  
Spectrum (Zoom)



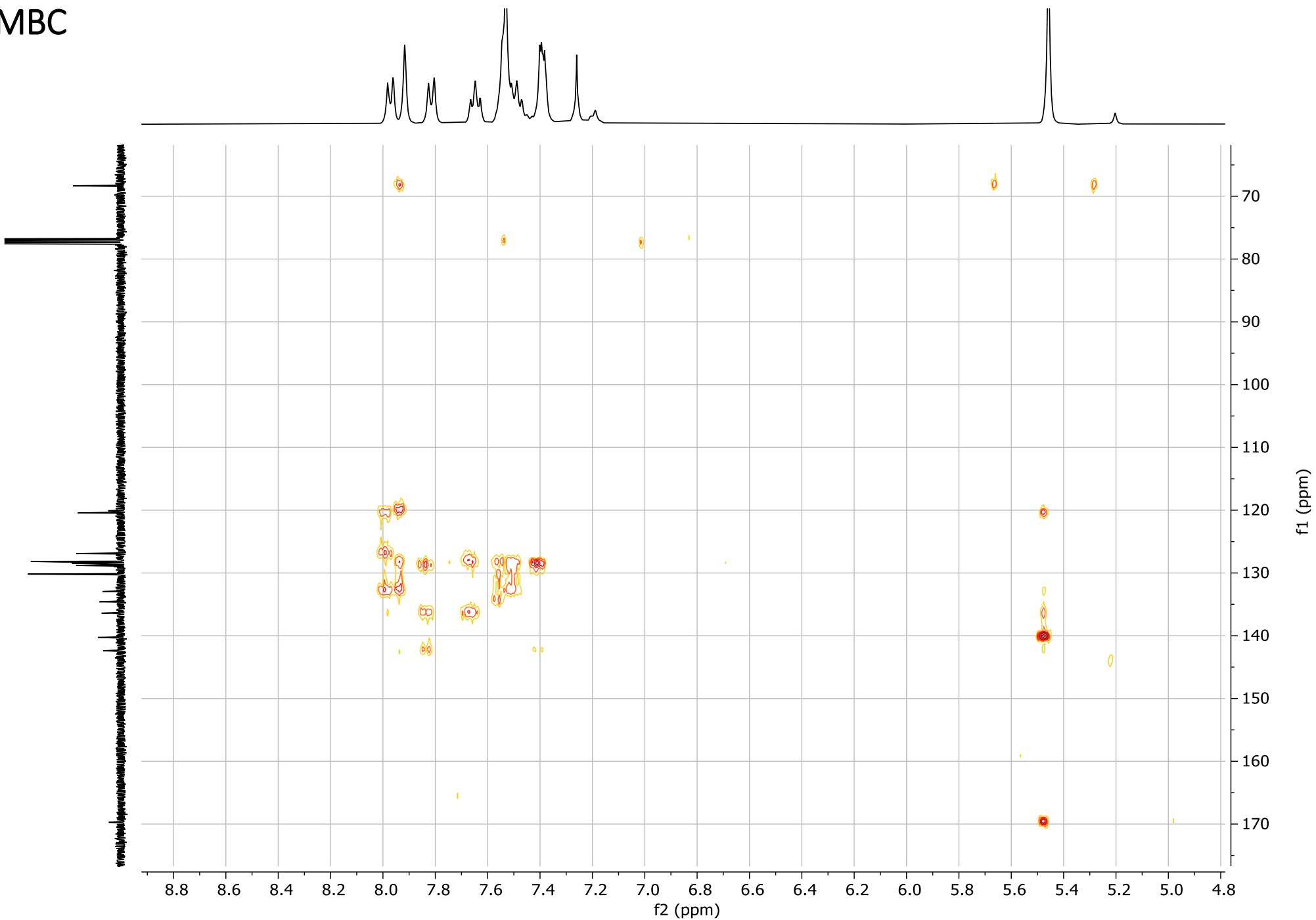
# Compound 2 – HSQC Spectrum



# Compound 2 – HSQC Spectrum (Zoom)

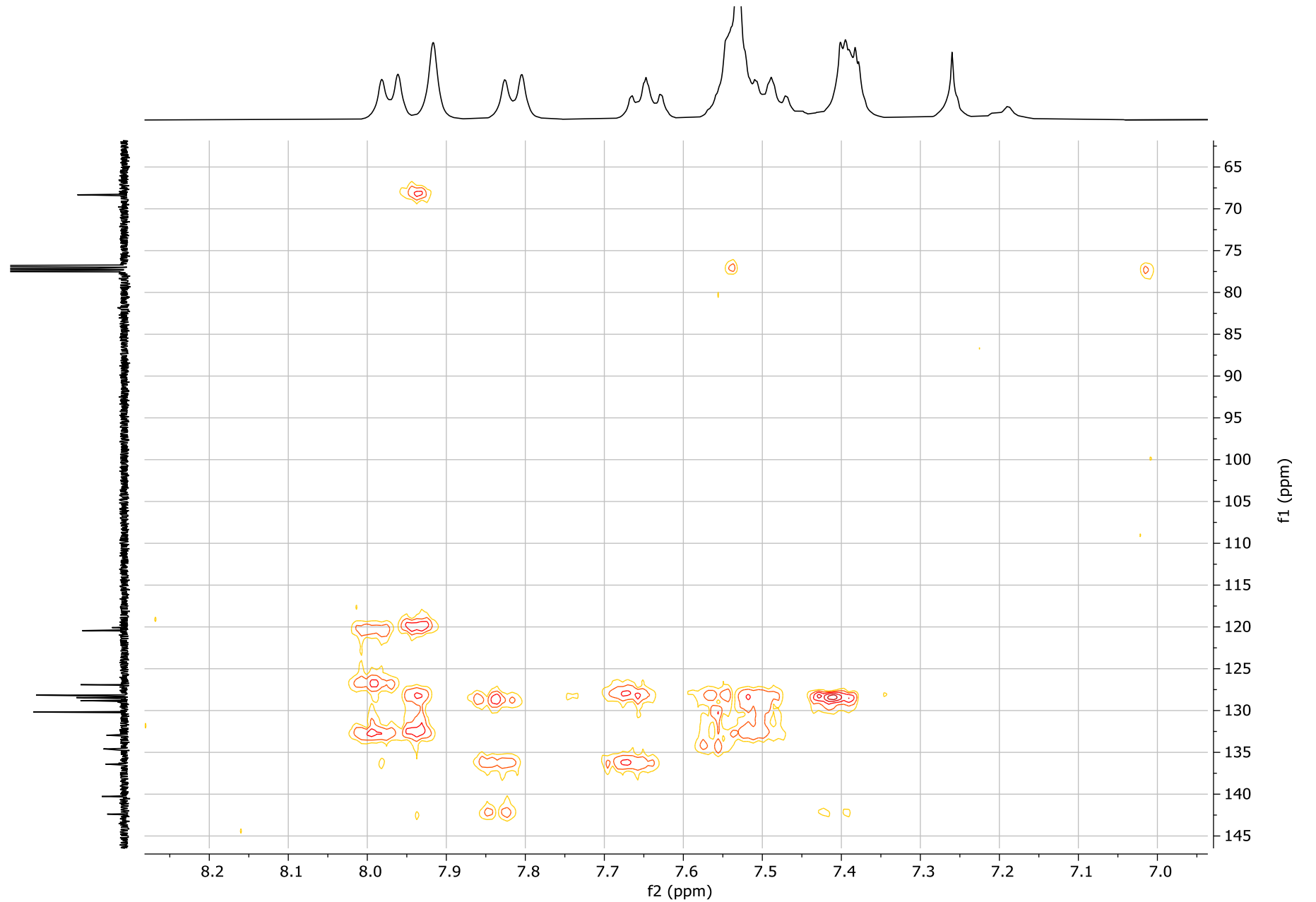


# Compound 2 – HMBC Spectrum

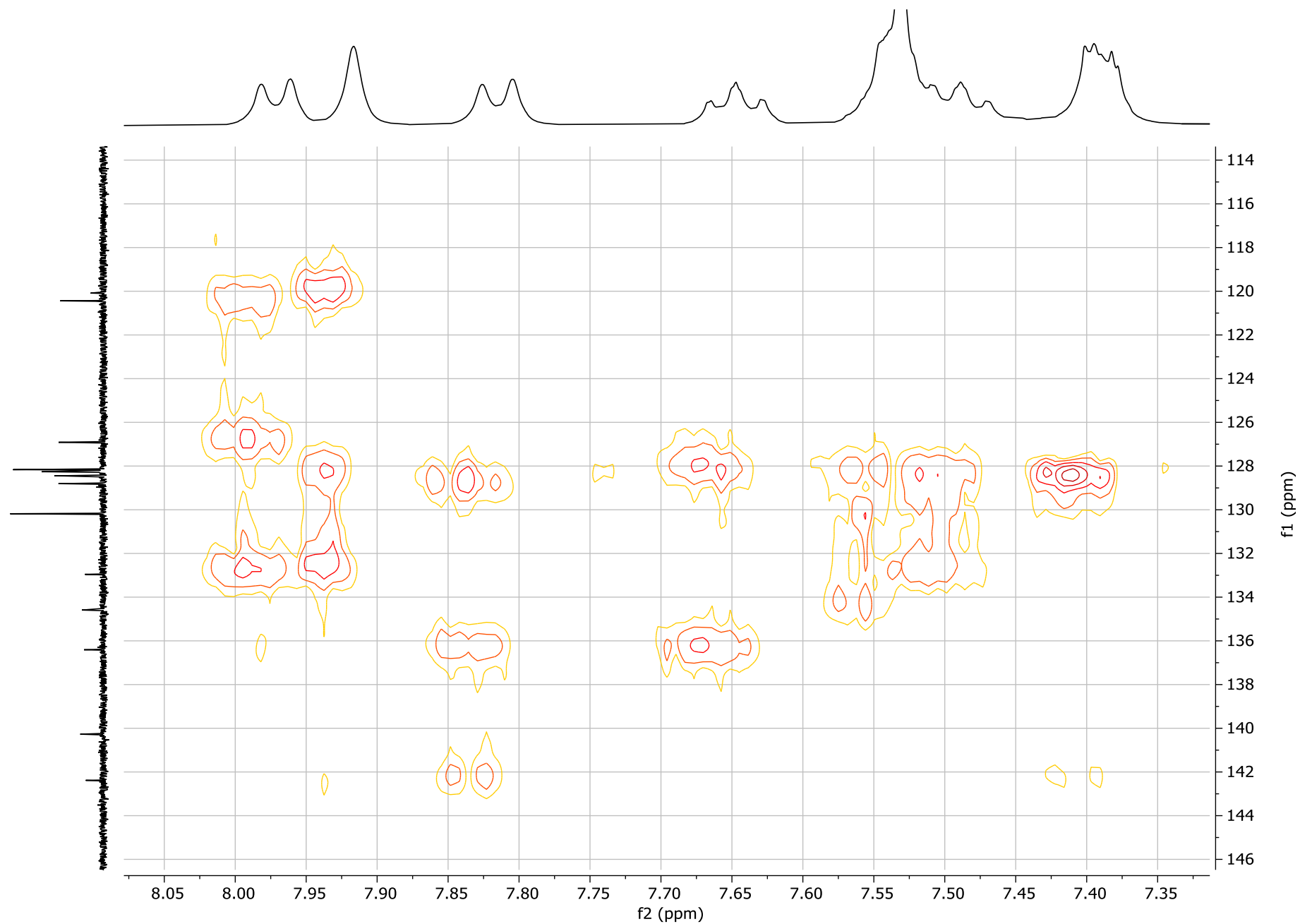




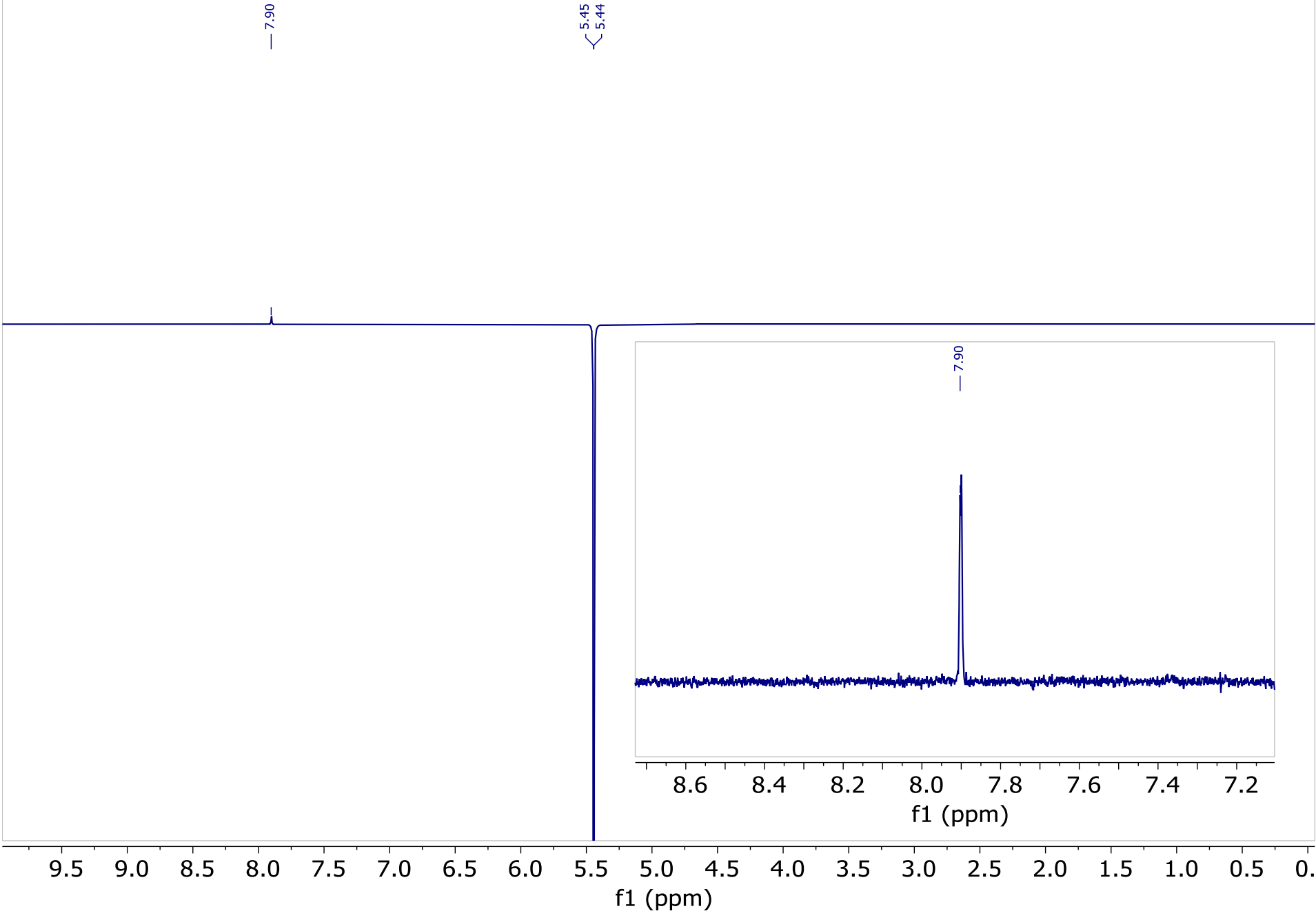
# Compound 2 – HMBC Spectrum (Zoom)



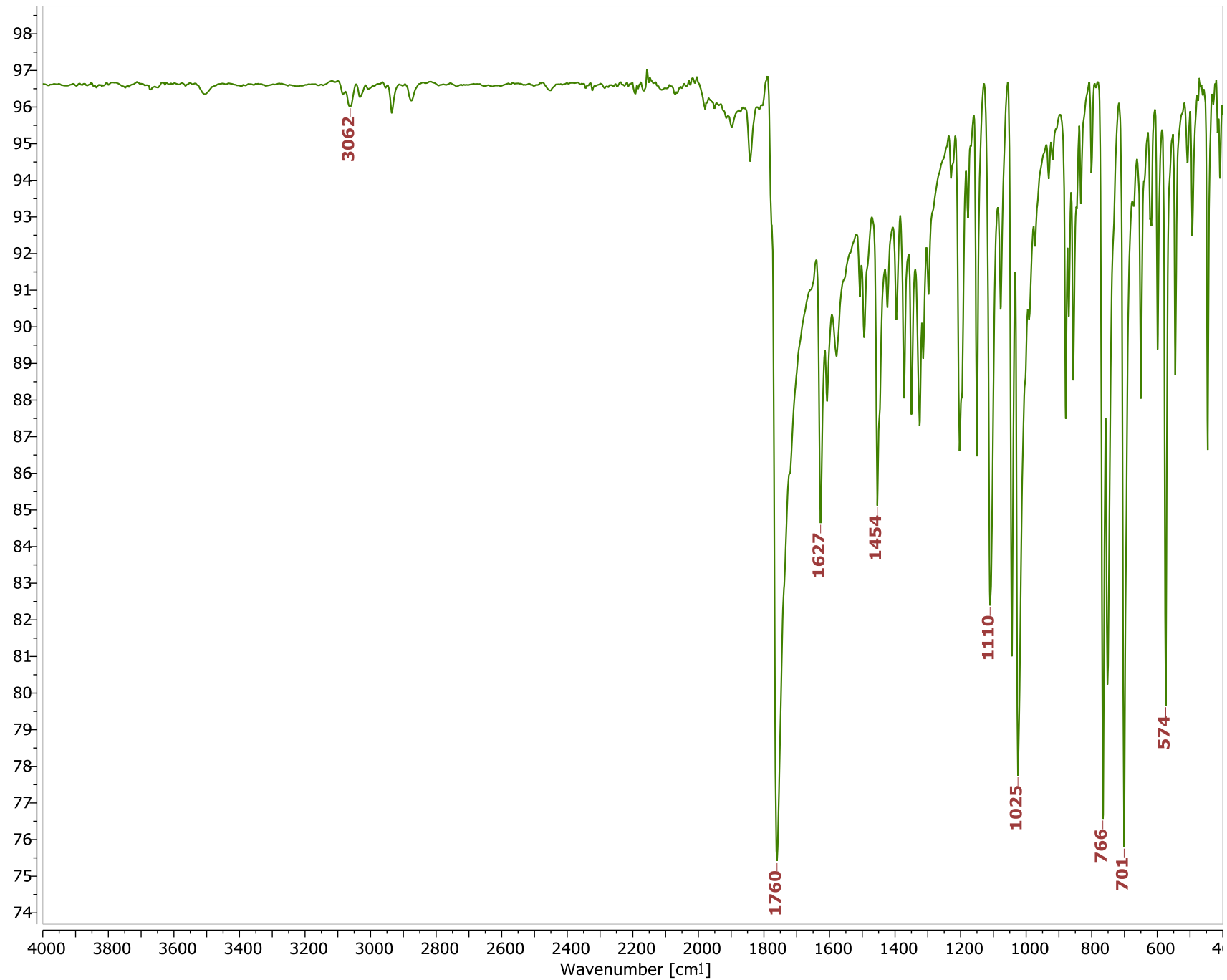
# Compound 2 – HMBC Spectrum (Zoom)



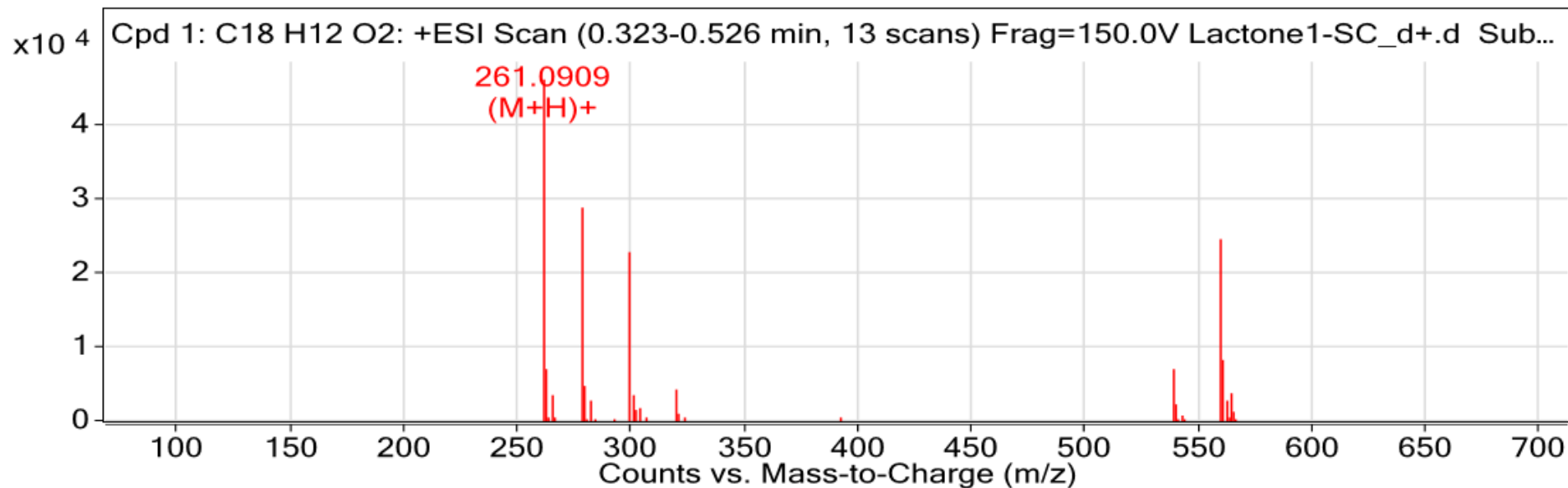
Compound 2 – 1D NOE  
Spectrum



# Compound 2 – IR Spectrum



# Compound 2 – Mass Spectrum



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
261.0909		46307	C18 H13 O2	(M+H)+
262.0945		7246	C18 H13 O2	(M+H)+
263.0974		763	C18 H13 O2	(M+H)+
265.1222		3690		
278.1175	1	29154	C18 H16 N O2	(M+NH4)+
279.1215	1	5112	C18 H16 N O2	(M+NH4)+
280.1258	1	479	C18 H16 N O2	(M+NH4)+
299.0472	1	23087	C18 H12 K O2	(M+K)+
300.0502	1	3665	C18 H12 K O2	(M+K)+
301.0471	1	1813	C18 H12 K O2	(M+K)+

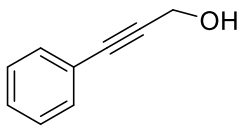
## Supplementary Material for Case Study # 2

### Can Slow, Steady and Green Get You the Correct Target?

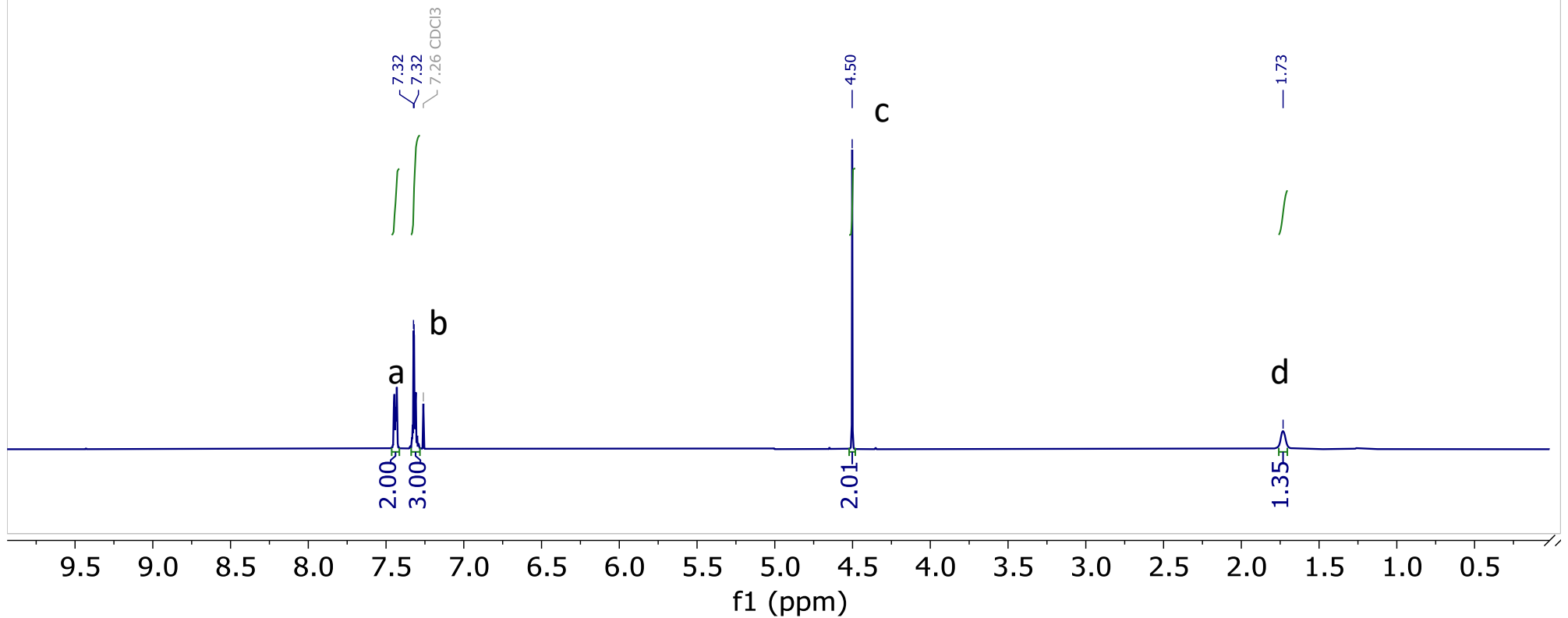
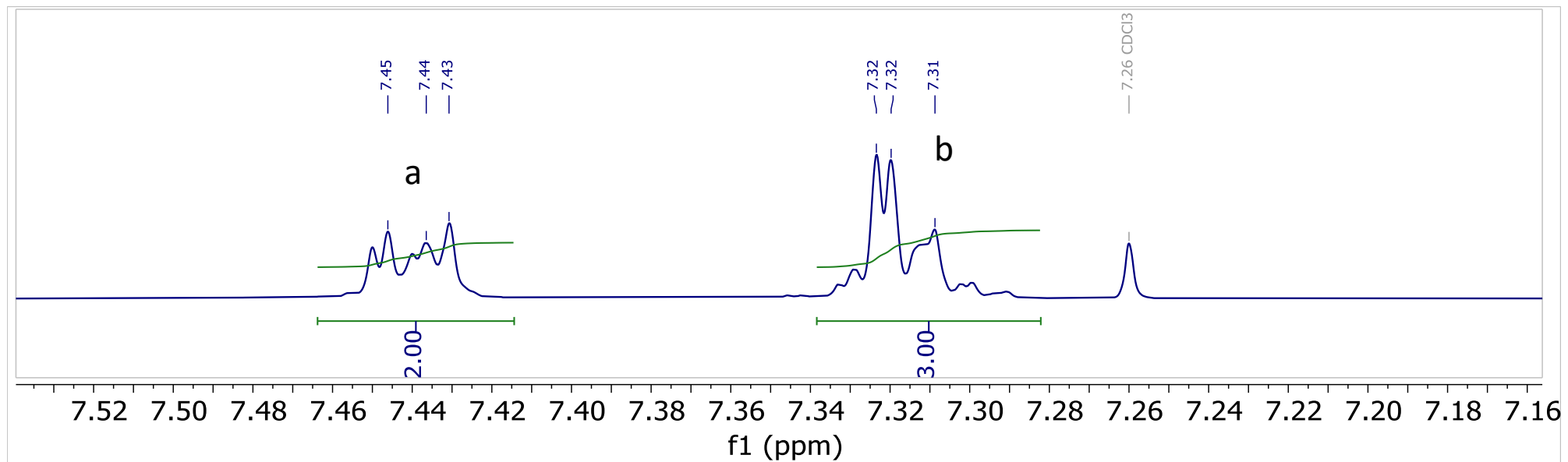
FIGURE	DESCRIPTION	PAGE
<b>S29</b>	3-Phenyl-2-propyn-1-ol - <sup>1</sup> H NMR	S29
<b>S30</b>	3-Phenyl-2-propyn-1-ol - <sup>13</sup> C NMR	S30
<b>S31</b>	3-Phenyl-2-propyn-1-ol - IR	S31
<b>S32</b>	Cinnamyl Alcohol - <sup>1</sup> H NMR	S32
<b>S33</b>	Cinnamyl Alcohol - <sup>13</sup> C NMR	S33
<b>S34</b>	Cinnamyl Alcohol - IR	S34
<b>S35</b>	Cinnamic Acid - <sup>1</sup> H NMR	S35
<b>S36</b>	Cinnamic Acid - <sup>13</sup> C NMR	S36
<b>S37</b>	Cinnamic Acid - IR	S37
<b>S38</b>	Phenyl Propiolic Acid - <sup>1</sup> H NMR	S38
<b>S39</b>	Phenyl Propiolic Acid - <sup>13</sup> C NMR	S39
<b>S40</b>	Phenyl Propiolic Acid - IR	S40
<b>S41</b>	Ester 1 - <sup>1</sup> H NMR	S41
<b>S42</b>	Ester 1 - <sup>13</sup> C NMR	S42
<b>S43</b>	Ester 1 - IR	S43
<b>S44</b>	Ester 2 - <sup>1</sup> H NMR	S44
<b>S45</b>	Ester 2 - <sup>13</sup> C NMR	S45
<b>S46</b>	Ester 2 - IR	S46
<b>S47</b>	Type 1 - <sup>1</sup> H NMR	S47

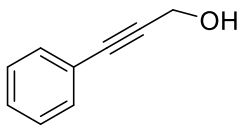
FIGURE	DESCRIPTION	PAGE
<b>S48</b>	Type 1 - <sup>13</sup> C NMR	S48
<b>S49</b>	Type 1 - APT	S49
<b>S50</b>	Type 1 - COSY	S50
<b>S51</b>	Type 1 - COSY (Zoom)	S51
<b>S52</b>	Type 1 - HSQC	S52
<b>S53</b>	Type 1 - HSQC (Zoom)	S53
<b>S54</b>	Type 1 - HMBC	S54
<b>S55</b>	Type 1 - HMBC (Zoom)	S55
<b>S56</b>	Type 1 - 1D NOE	S56
<b>S57</b>	Type 1 - IR	S57
<b>S58</b>	Type 1 - Mass Spectrum	S58
<b>S59</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - <sup>1</sup> H NMR	S59
<b>S60</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - <sup>13</sup> C NMR	S60
<b>S61</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - COSY	S61
<b>S62</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - COSY (Zoom)	S62
<b>S63</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - COSY (Zoom)	S63
<b>S64</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - HSQC	S64
<b>S65</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - HSQC (Zoom)	S65
<b>S66</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - HSQC (Zoom)	S66

FIGURE	DESCRIPTION	PAGE
<b>S67</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - HMBC	S67
<b>S68</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - HMBC (Zoom)	S68
<b>S69</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - HMBC (Zoom)	S69
<b>S70</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - DEPT-135	S70
<b>S71</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - IR	S71
<b>S72</b>	C <sub>18</sub> H <sub>14</sub> O <sub>2</sub> - Mass Spectrum	S72
<b>S73</b>	Type 2 - <sup>1</sup> H NMR	S73
<b>S74</b>	Type 2 - <sup>13</sup> C NMR	S74
<b>S75</b>	Type 2 - APT	S75
<b>S76</b>	Type 2 - COSY	S76
<b>S77</b>	Type 2 - COSY (Zoom)	S77
<b>S78</b>	Type 2 - HSQC	S78
<b>S79</b>	Type 2 - HSQC (Zoom)	S79
<b>S80</b>	Type 2 - HMBC	S80
<b>S81</b>	Type 2 - HMBC (Zoom)	S81
<b>S82</b>	Type 2 - HMBC (Zoom)	S82
<b>S83</b>	Type 2 - 1D NOE	S83
<b>S84</b>	Type 2 - IR	S84
<b>S85</b>	Type 2 - Mass Spectrum	S85
<b>S86</b>	DSC	S86

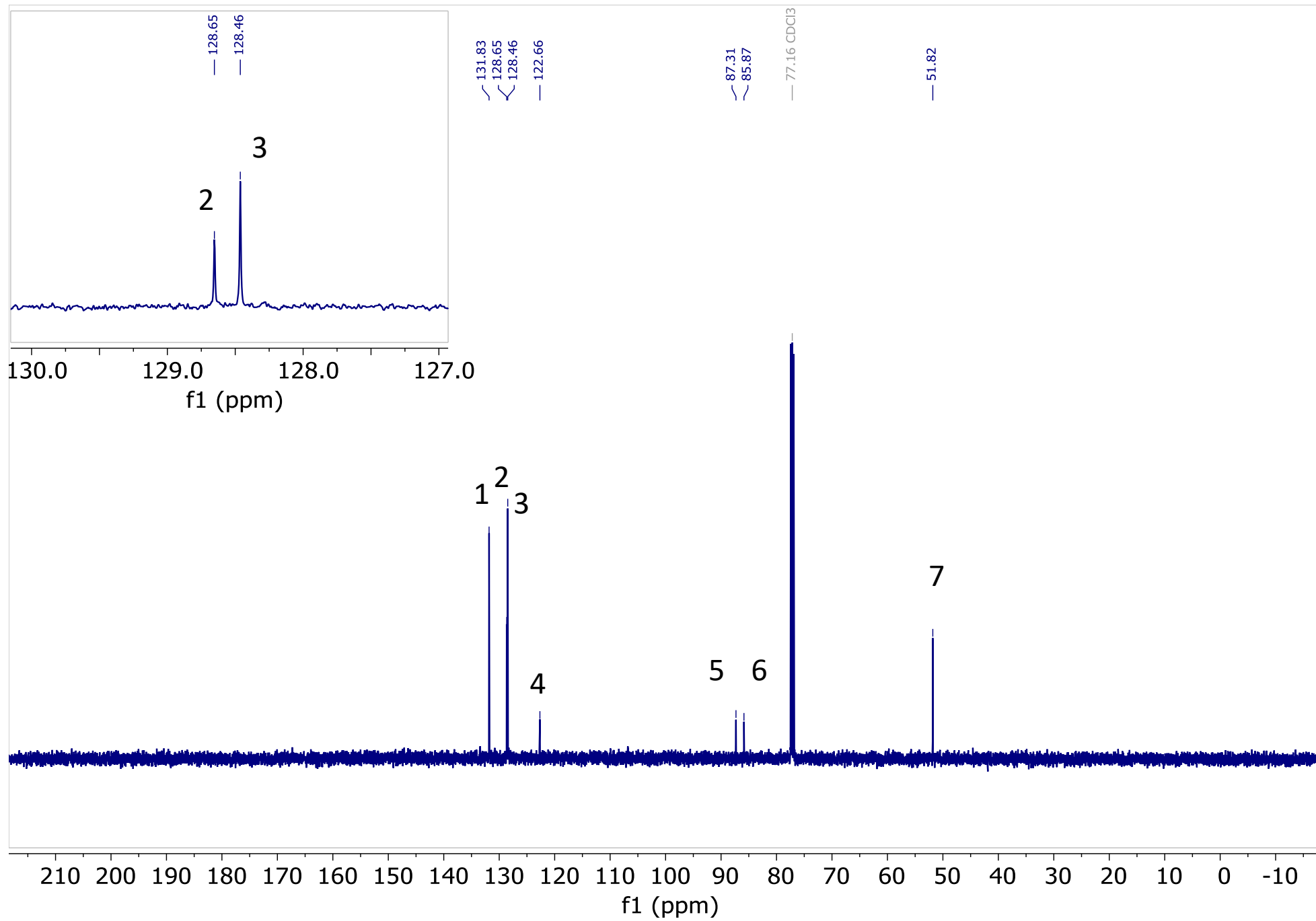


3-Phenyl-2-propyn-1-ol  
<sup>1</sup>H NMR

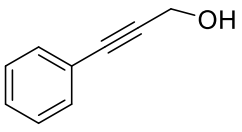




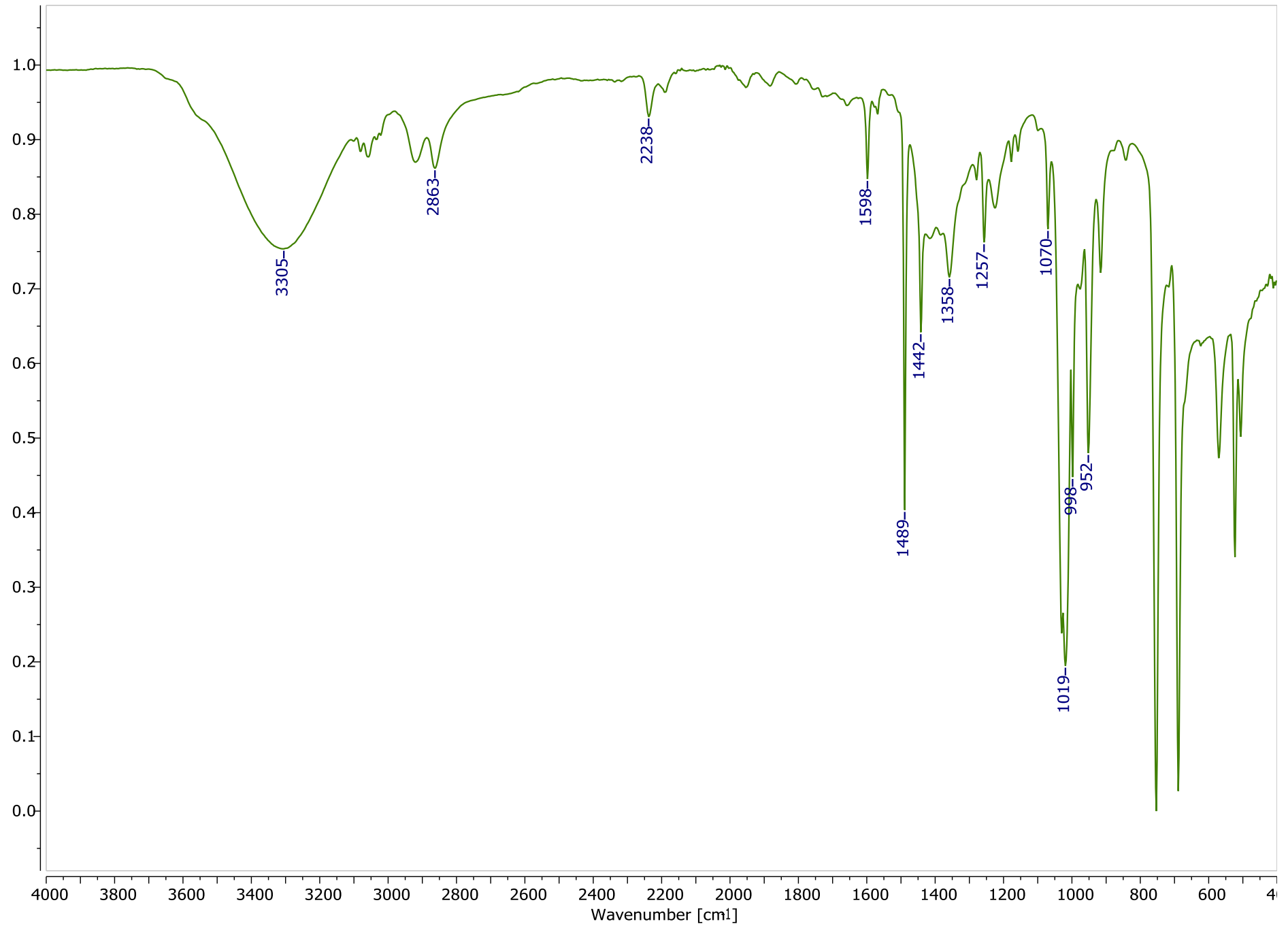
3-Phenyl-2-propyn-1-ol  
<sup>13</sup>C NMR

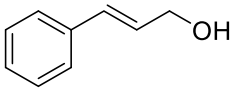




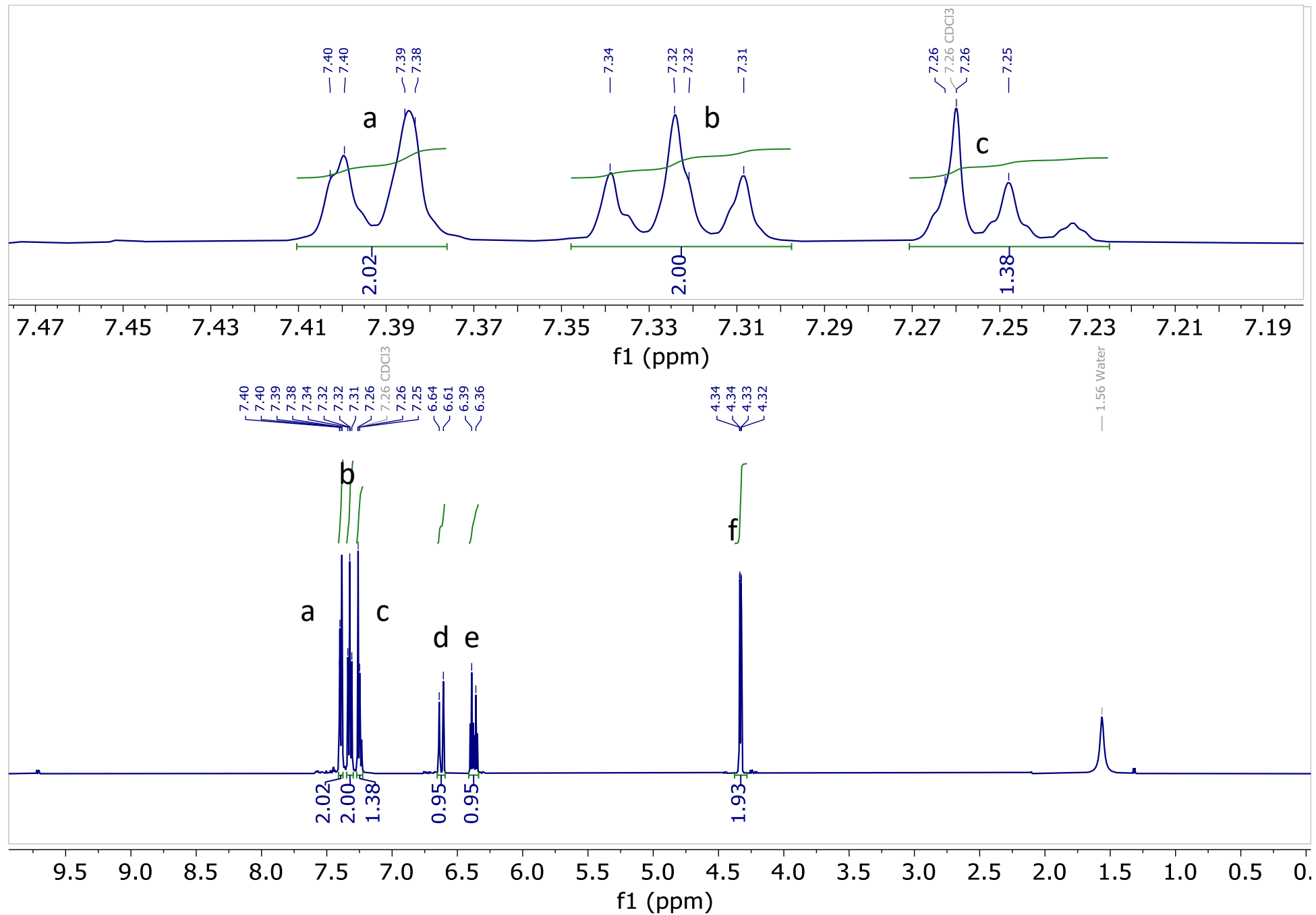


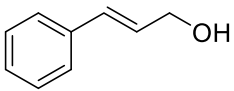
3-Phenyl-2-propyn-1-ol  
ATR



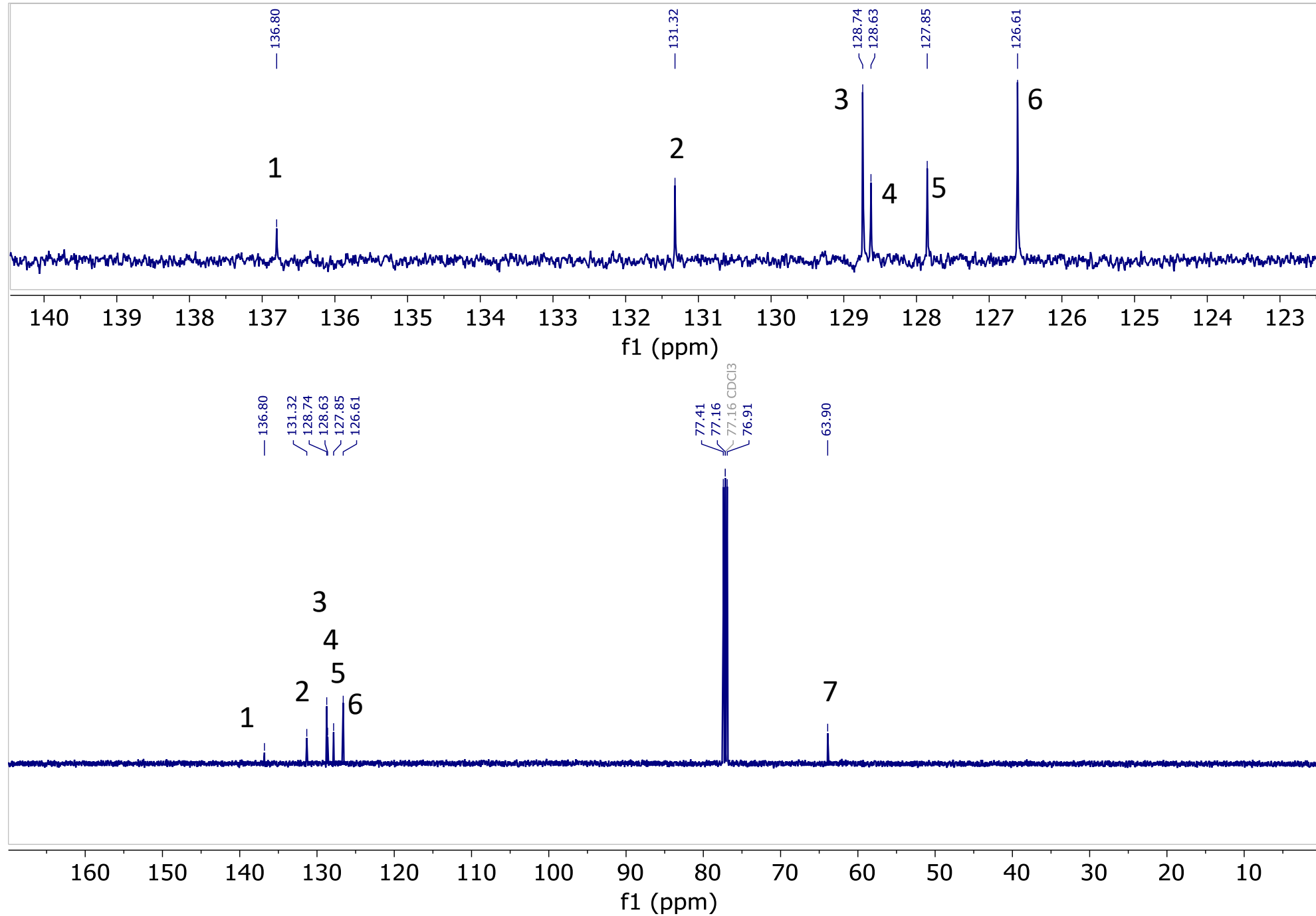


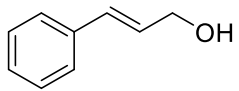
Cinnamyl Alcohol  
 $^1\text{H}$  NMR



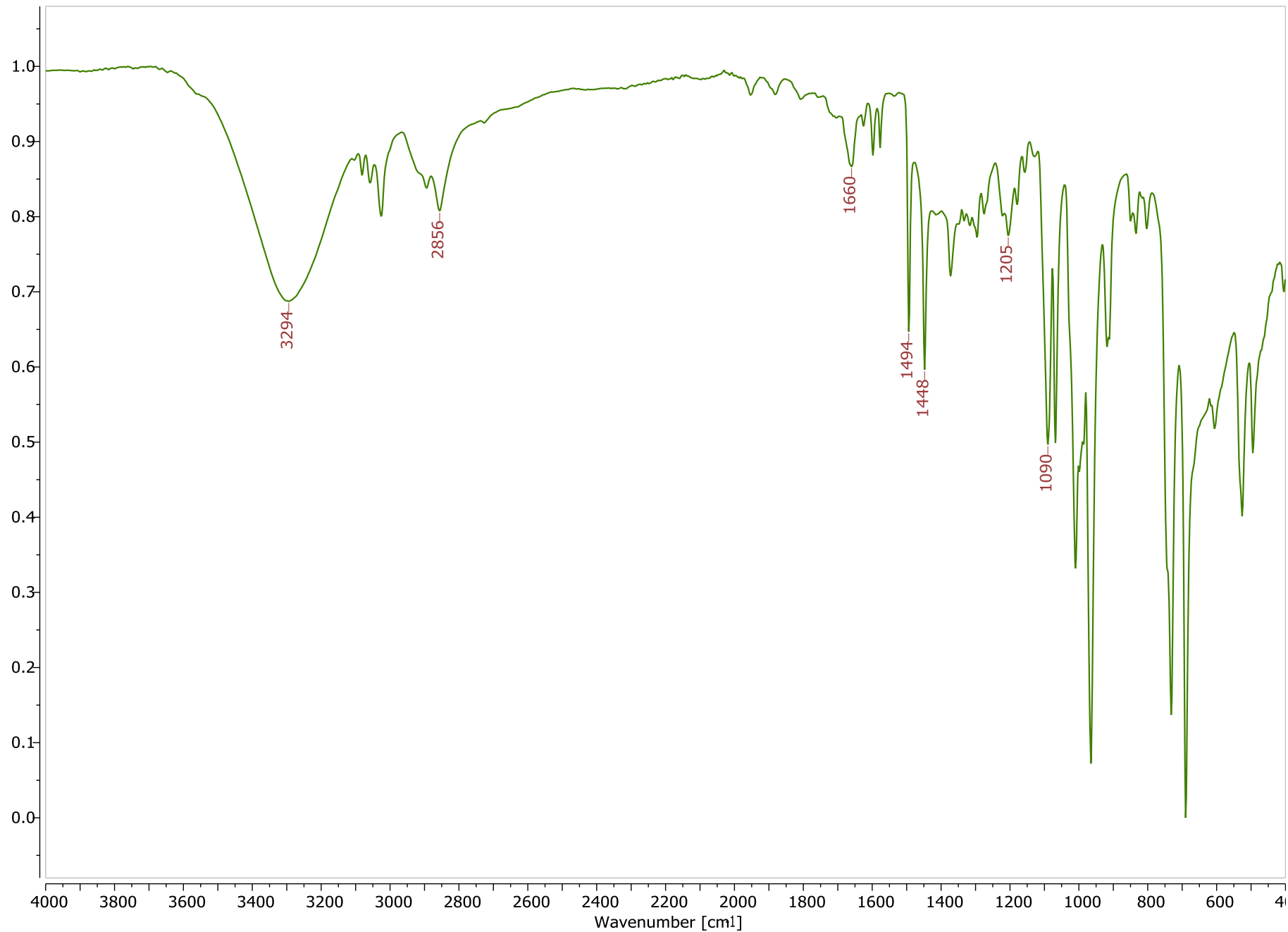


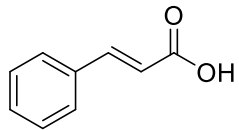
Cinnamyl Alcohol  
<sup>13</sup>C NMR



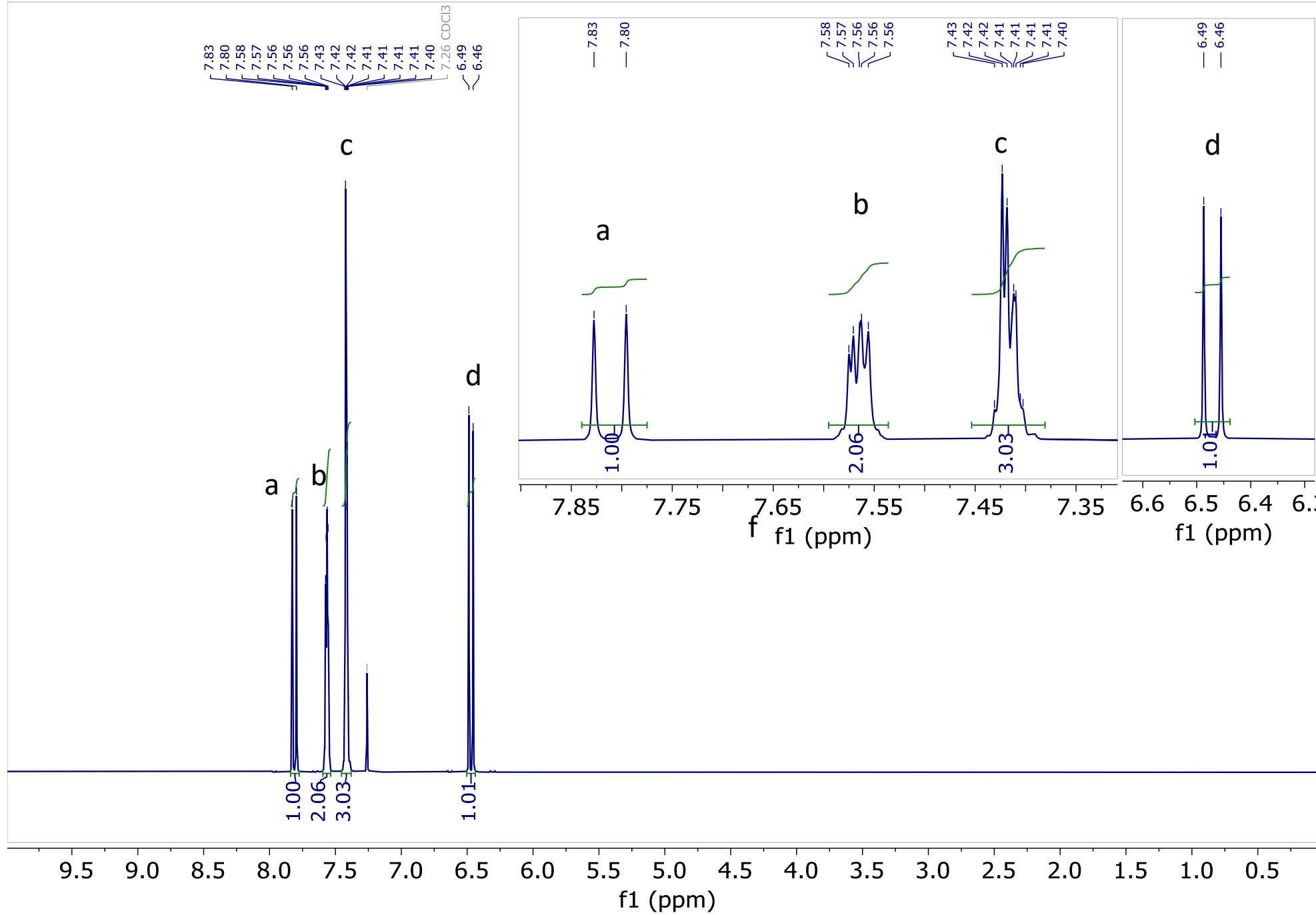


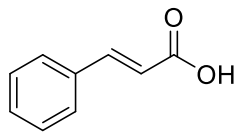
Cinnamyl Alcohol  
ATR





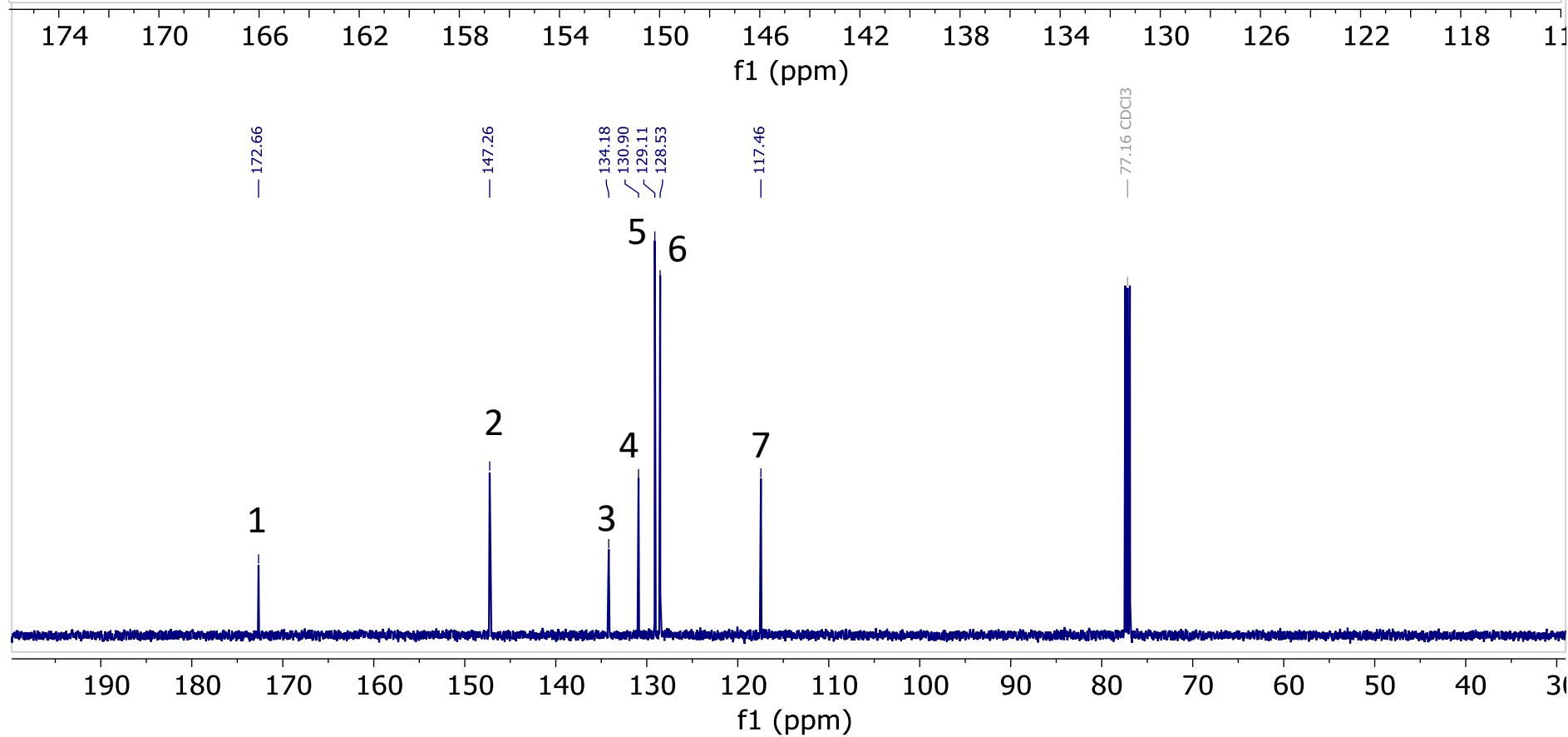
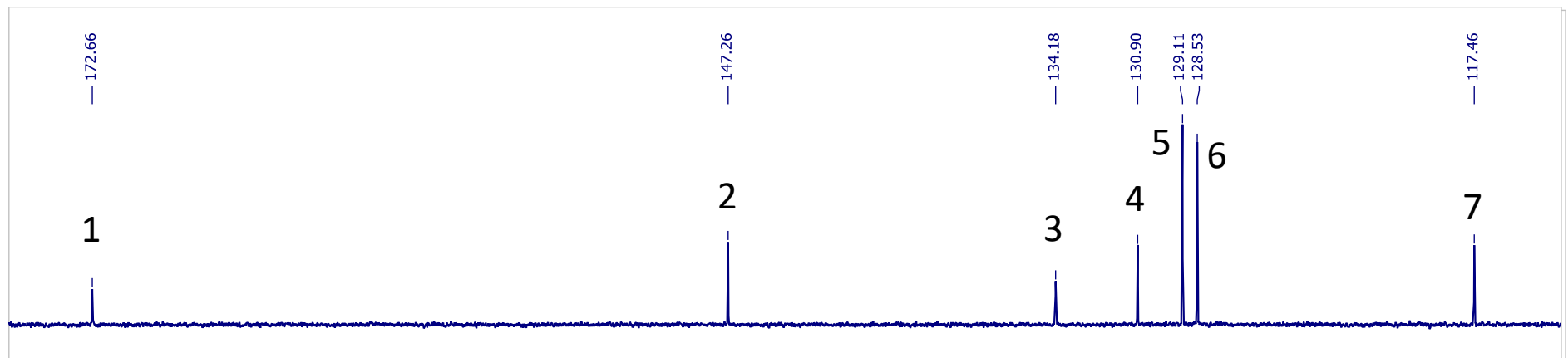
Cinnamic Acid  
 $^1\text{H}$  NMR

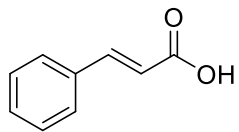




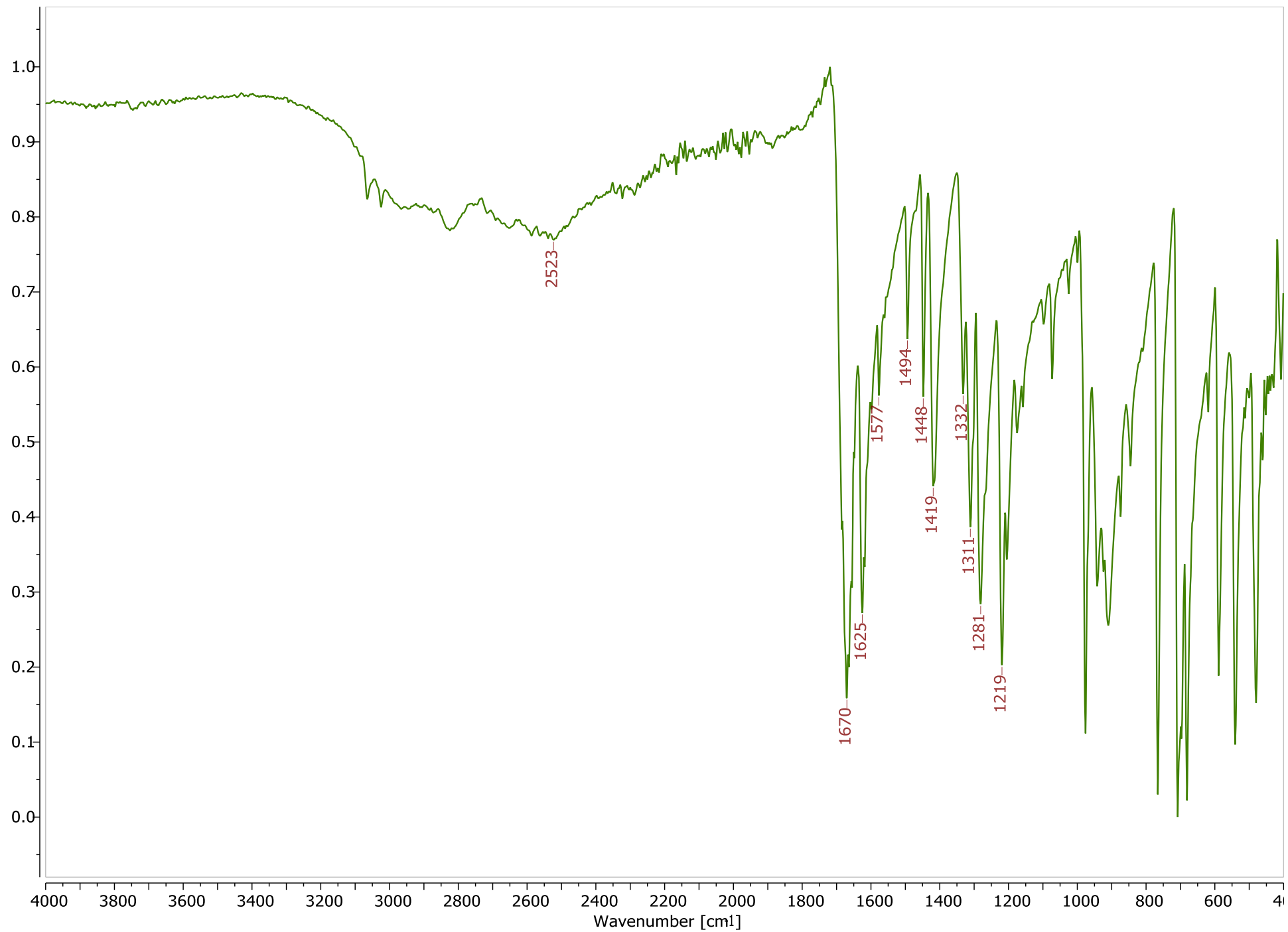
Cinnamic Acid

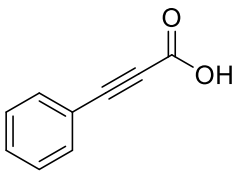
$^{13}\text{C}$  NMR



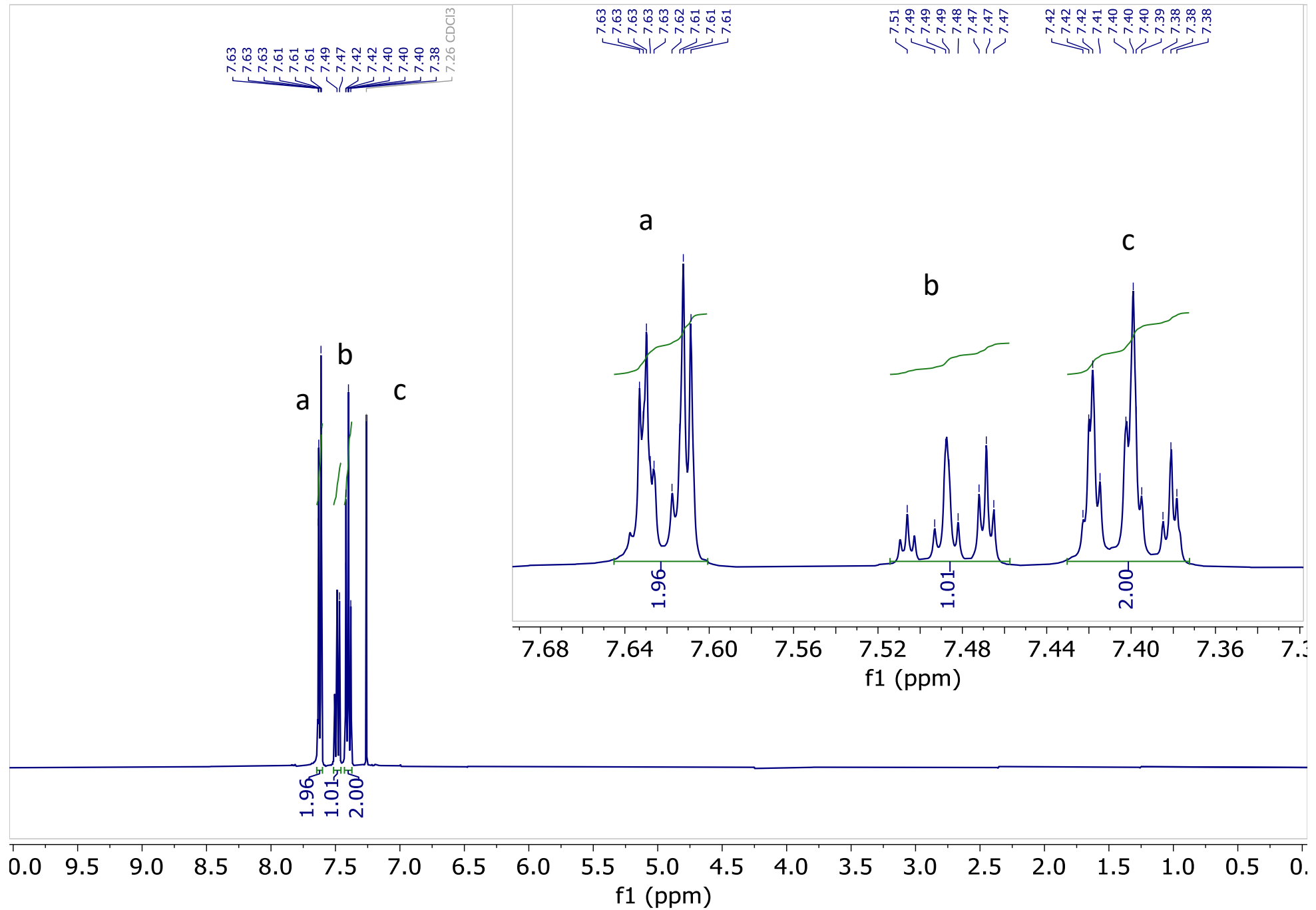


Cinnamic Acid  
ATR

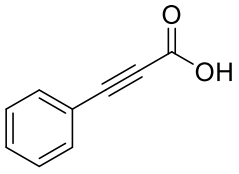




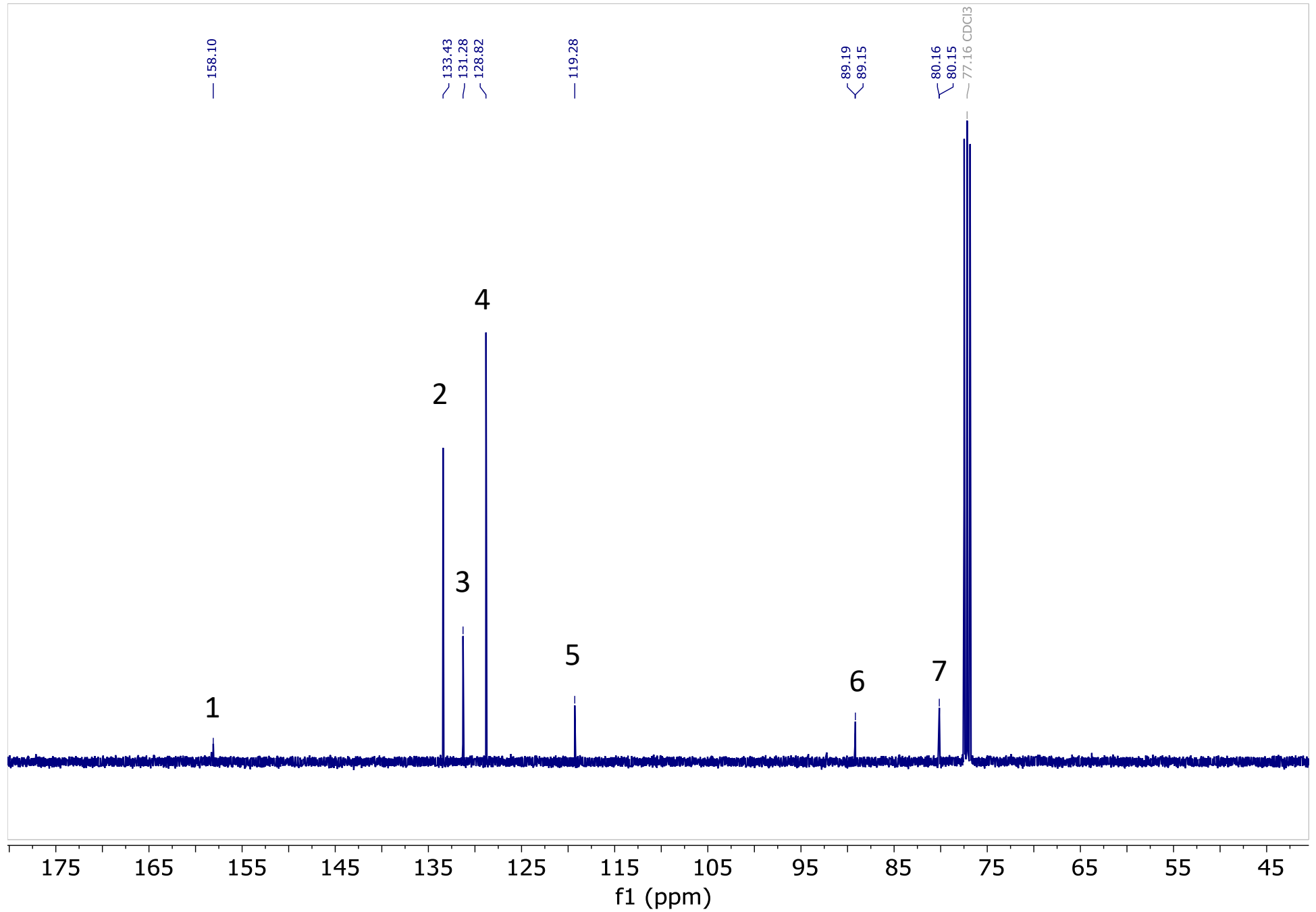
Phenyl Propiolic Acid  
 $^1\text{H}$  NMR

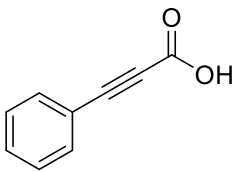




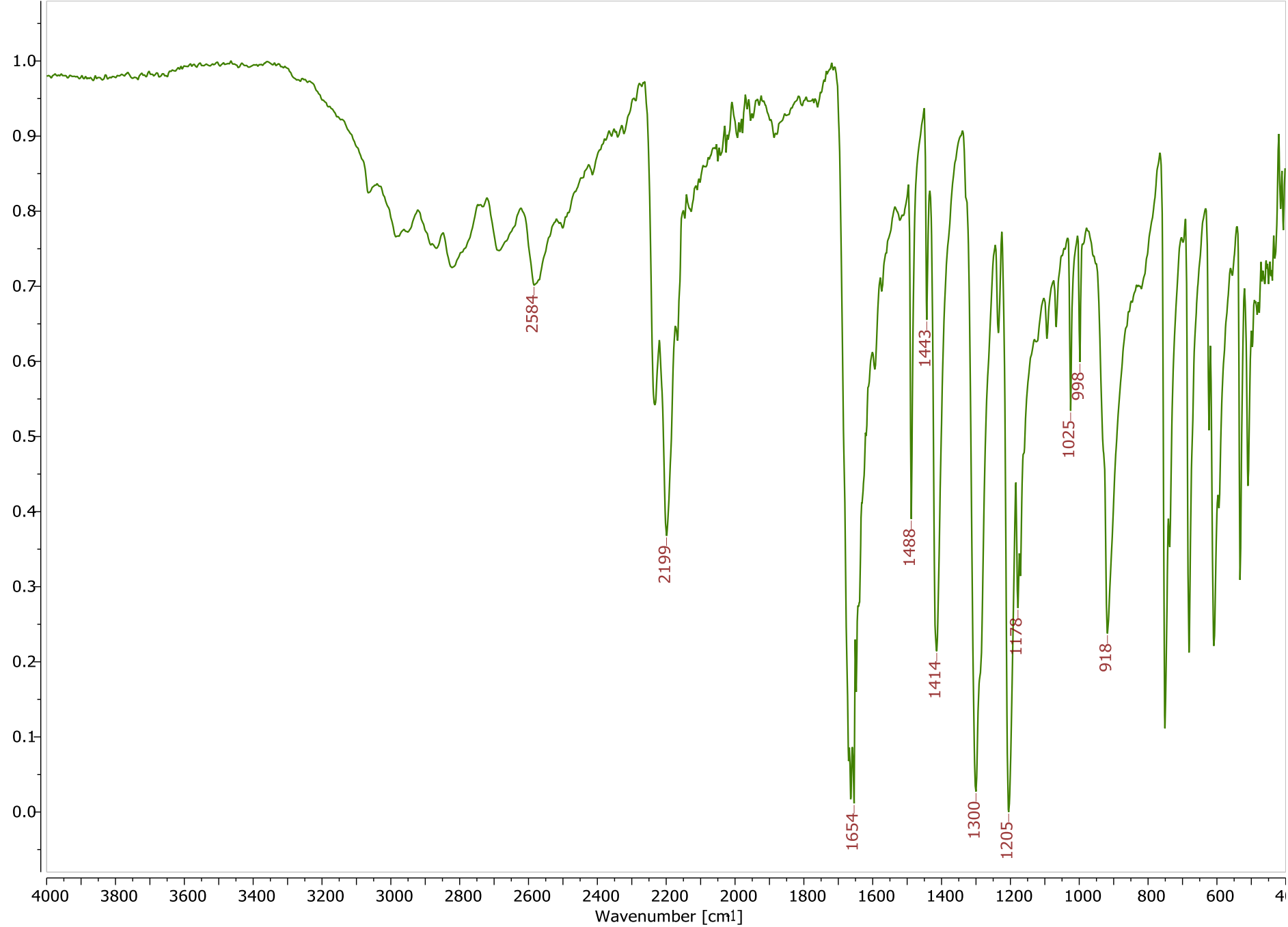


Phenyl Propiolic Acid  
<sup>13</sup>C NMR

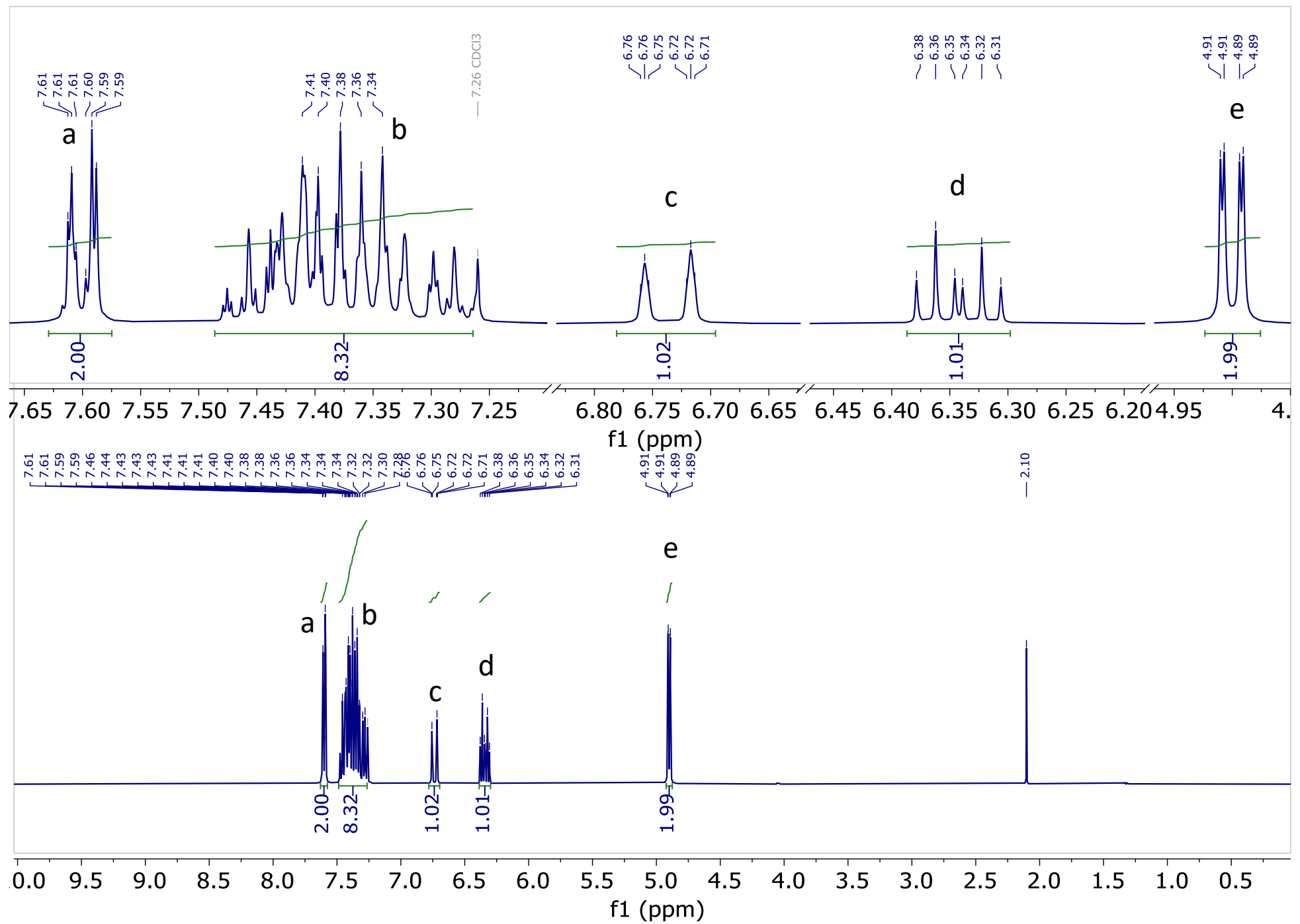




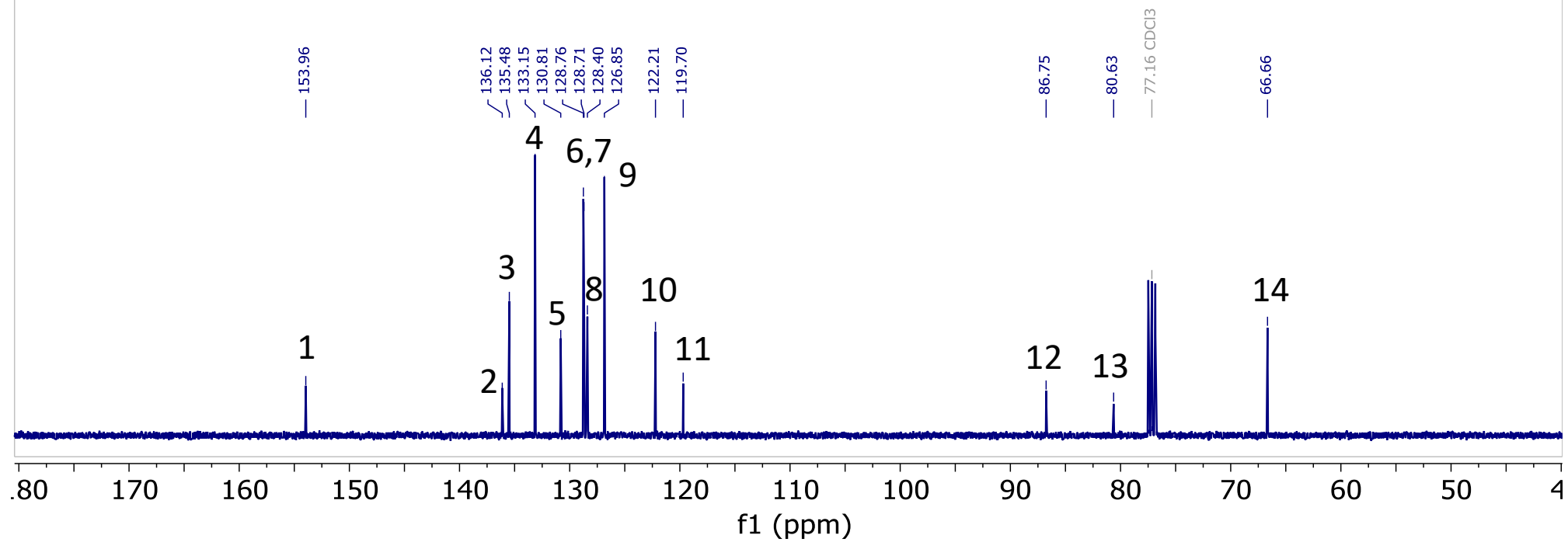
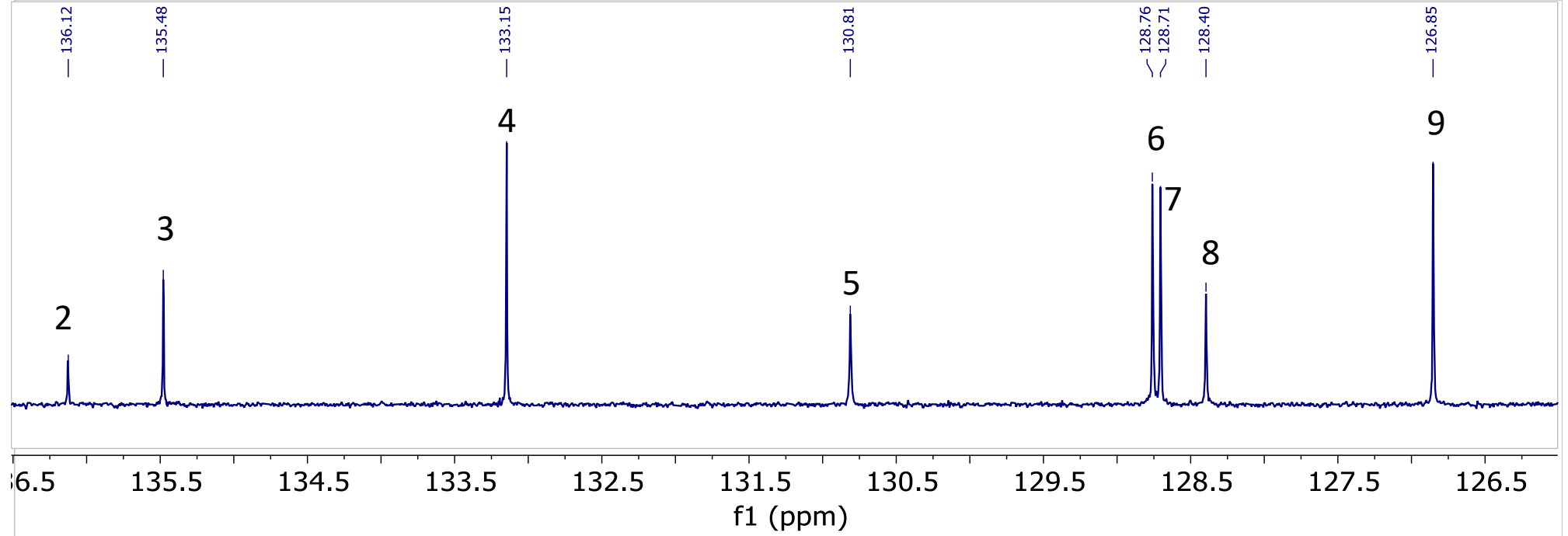
Phenyl Propiolic Acid  
ATR



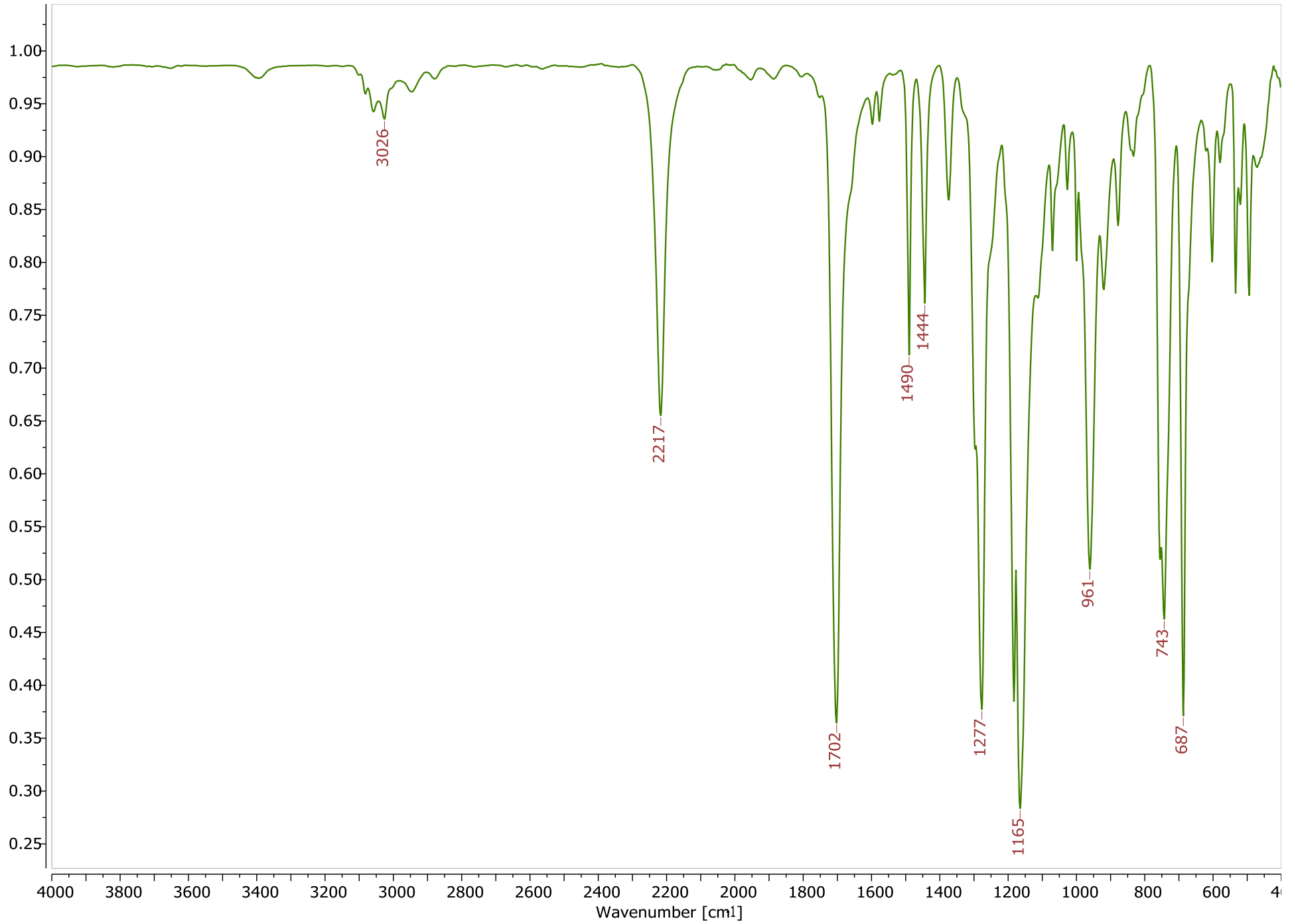
Ester 1  
<sup>1</sup>H NMR



Ester 1  
<sup>13</sup>C NMR

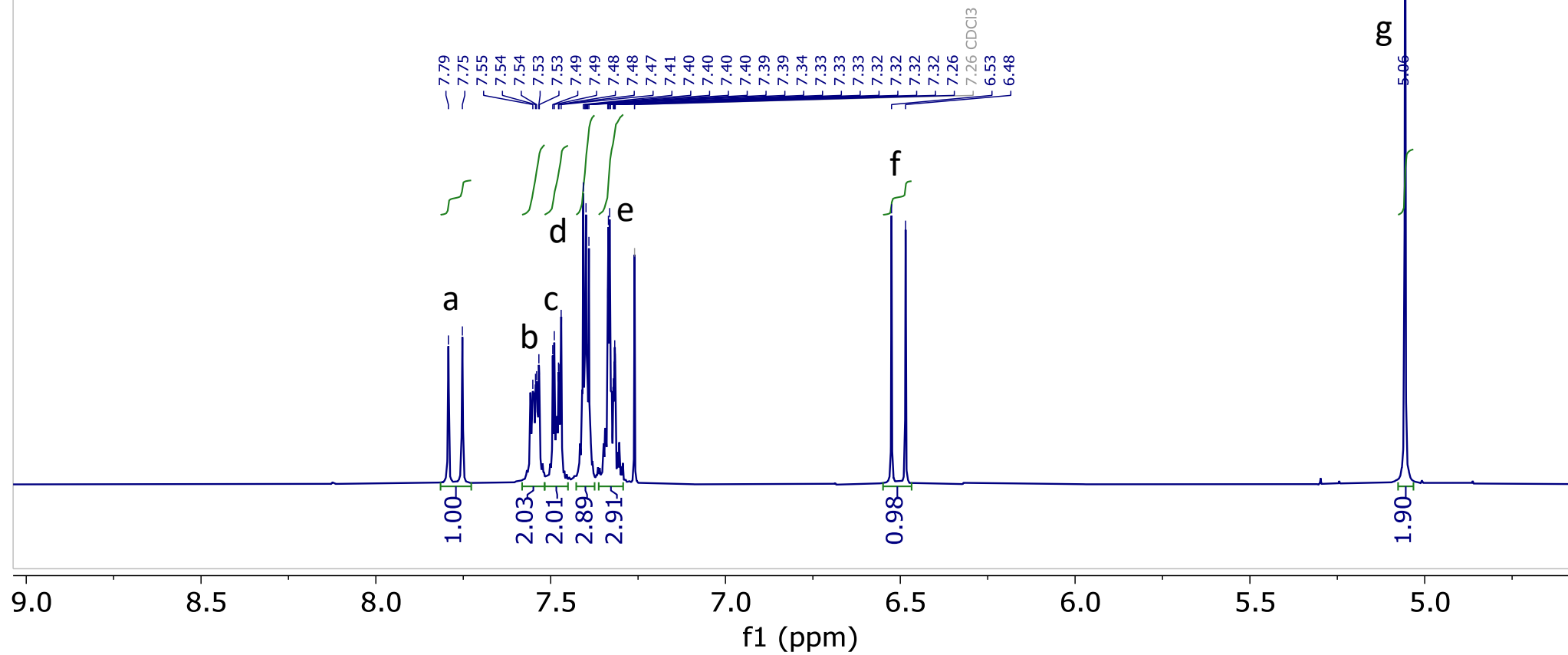
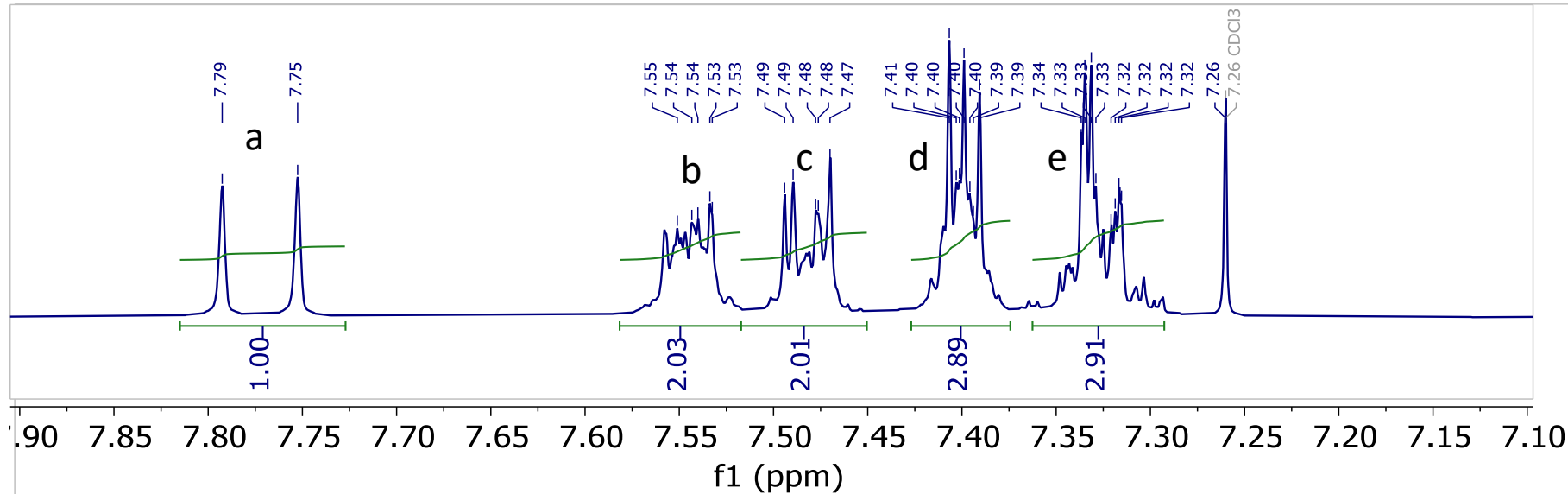


Ester 1  
ATR

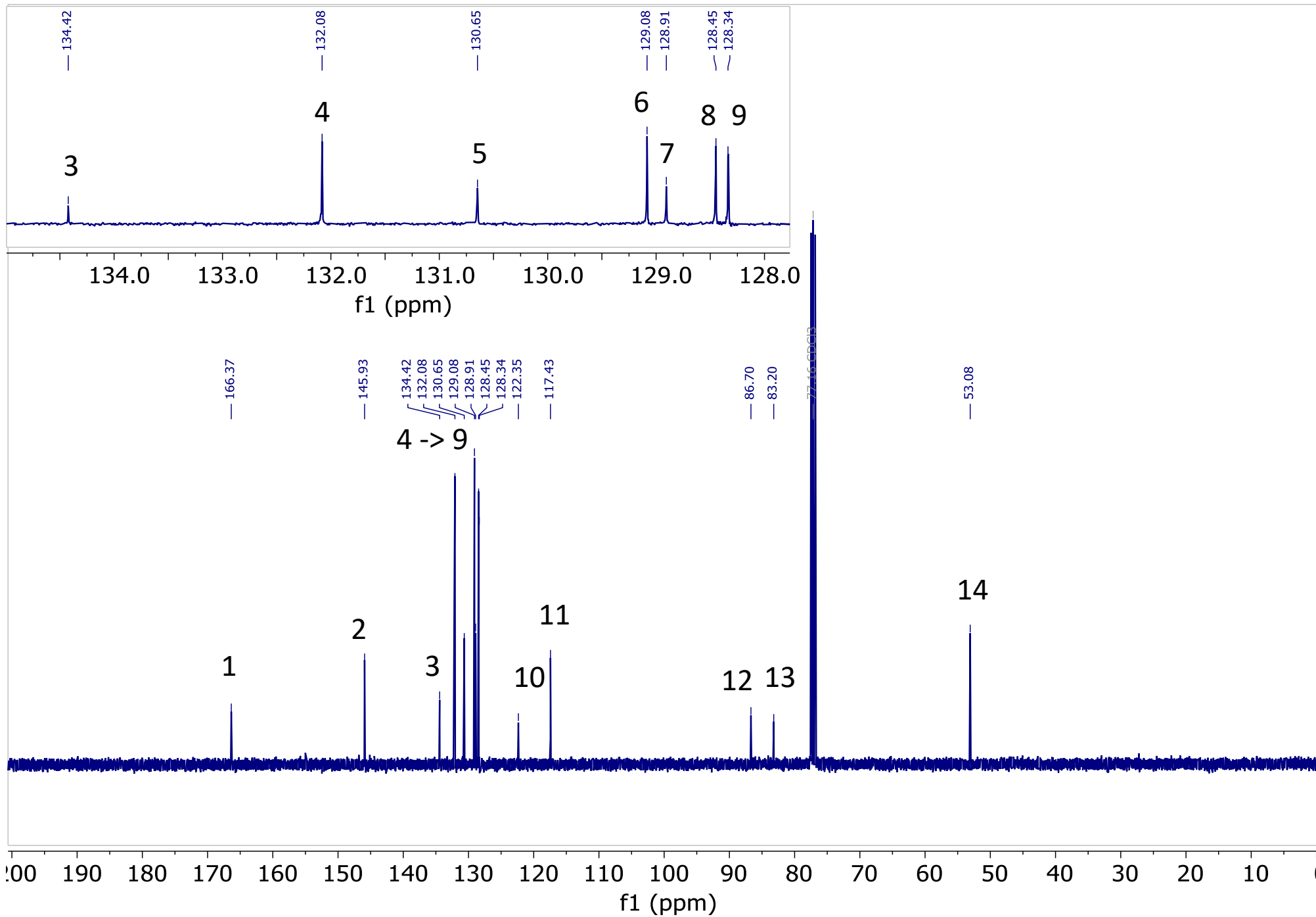


S43

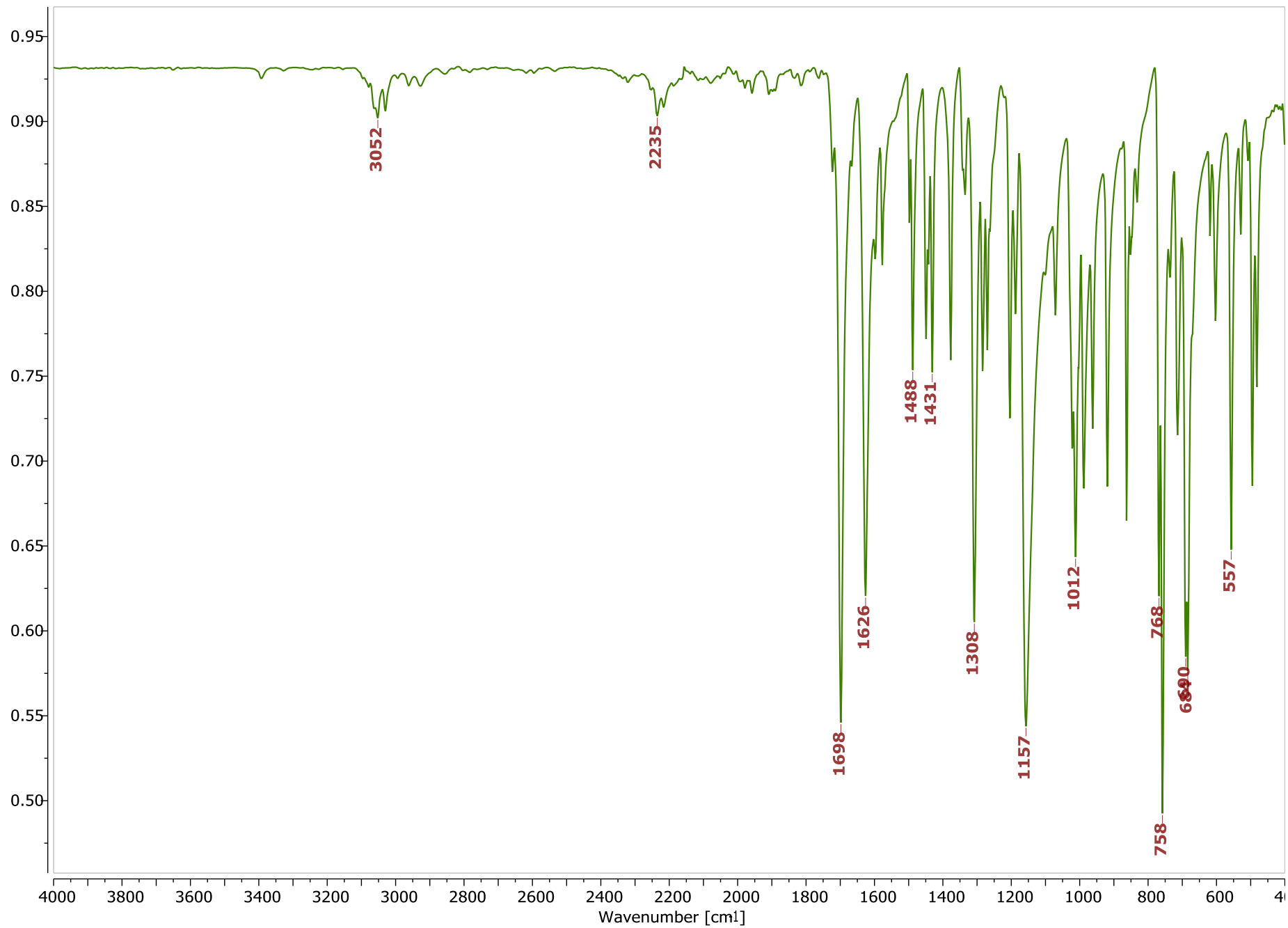
Ester 2  
<sup>1</sup>H NMR



Ester 2  
<sup>13</sup>C NMR



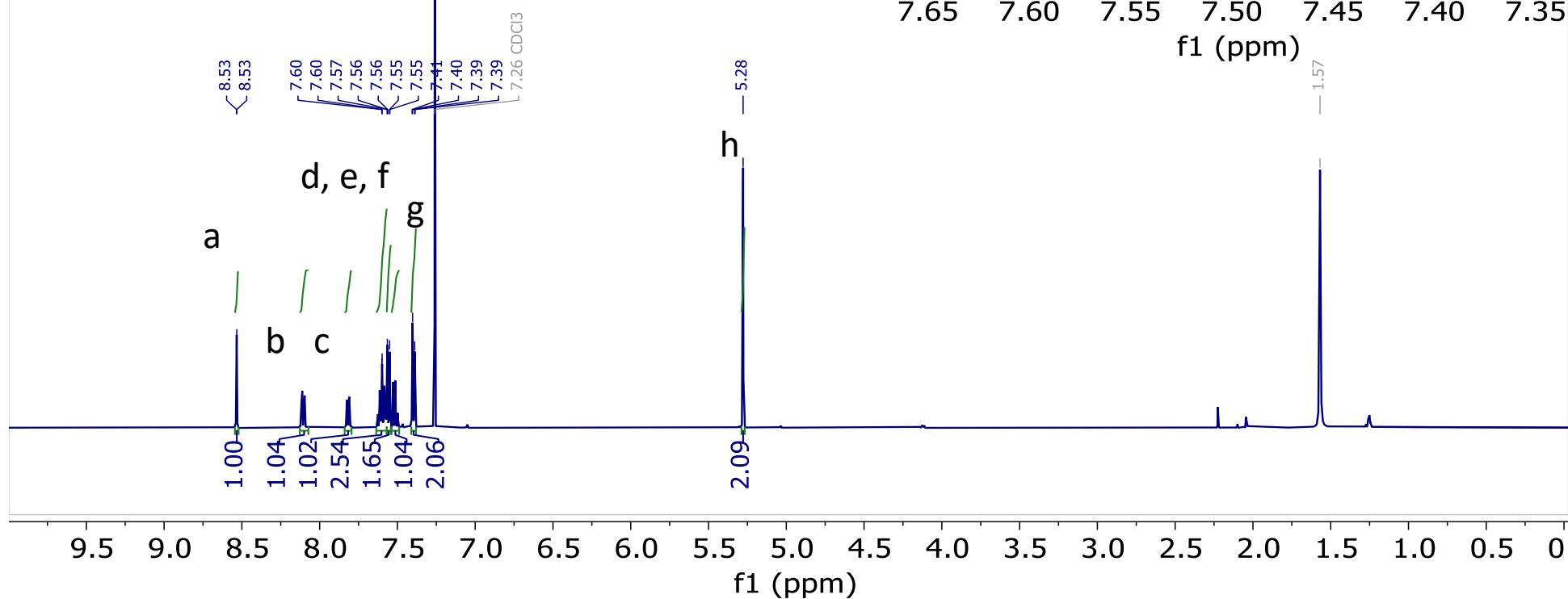
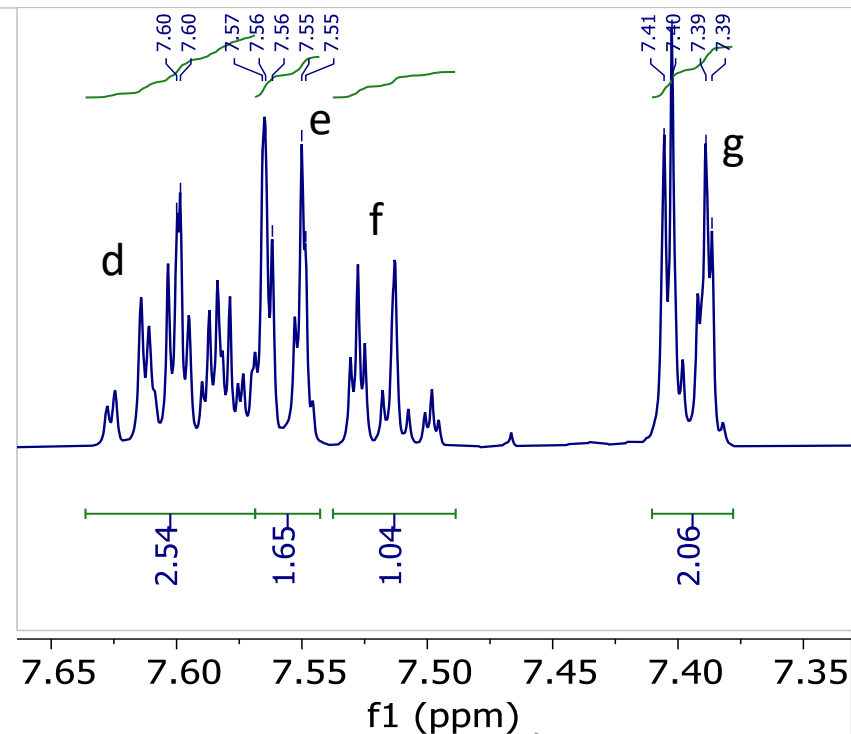
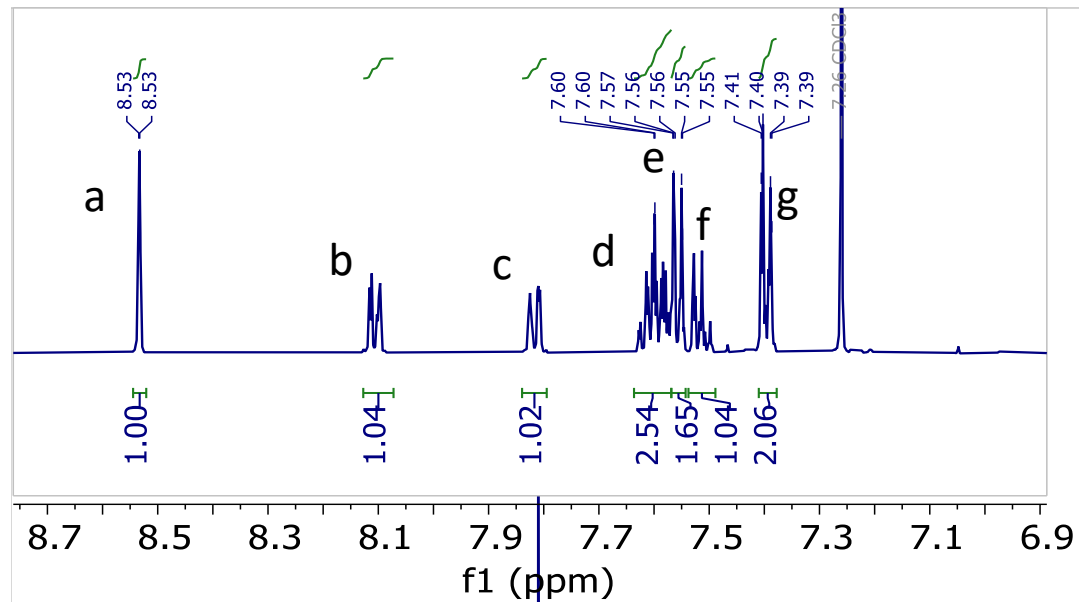
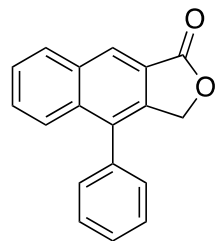
Ester 2  
ATR



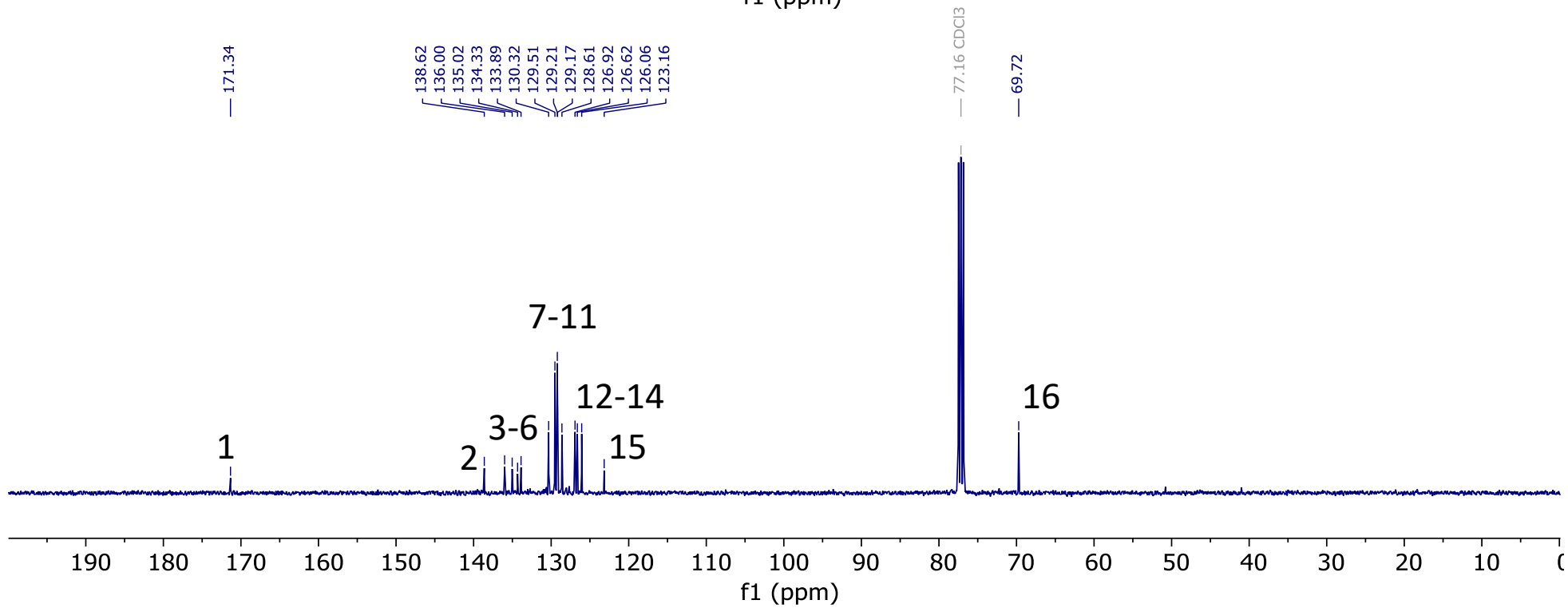
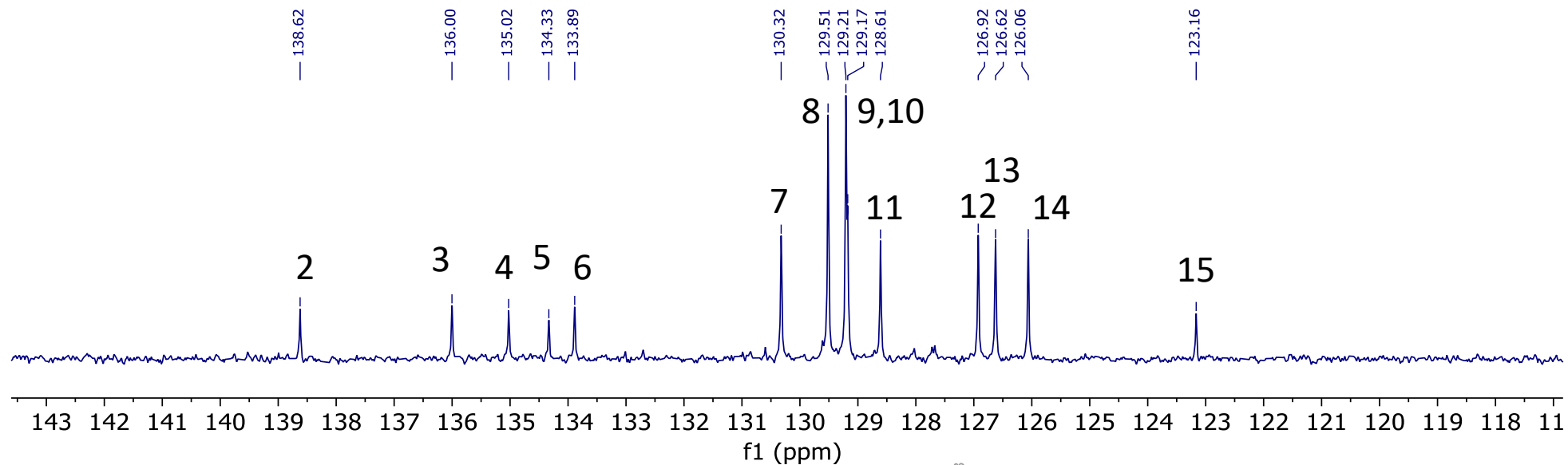
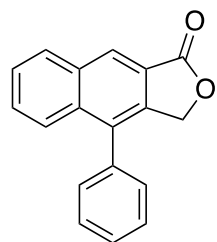
S46



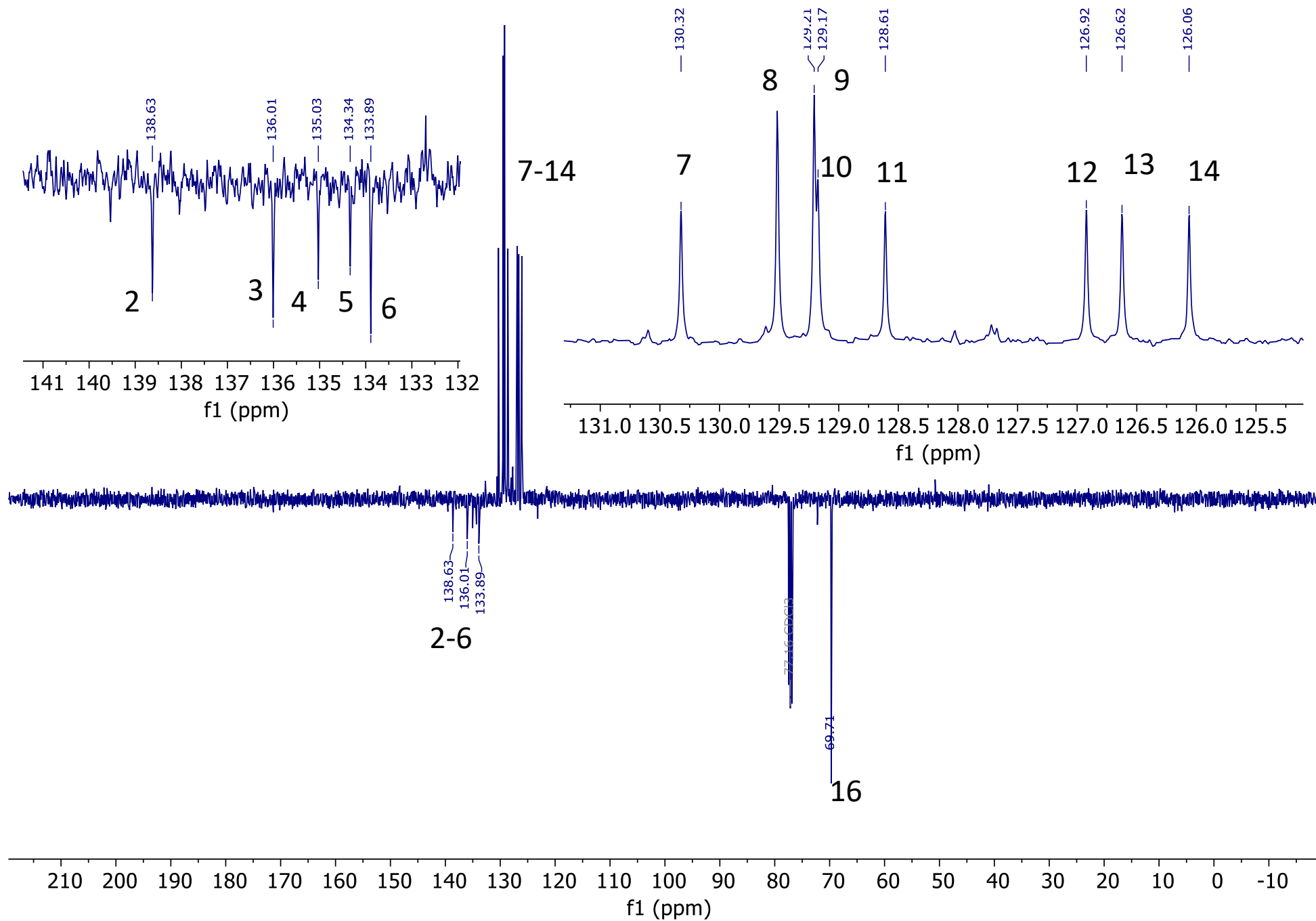
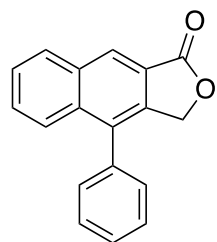
# Type 1 – <sup>1</sup>H-NMR Spectrum



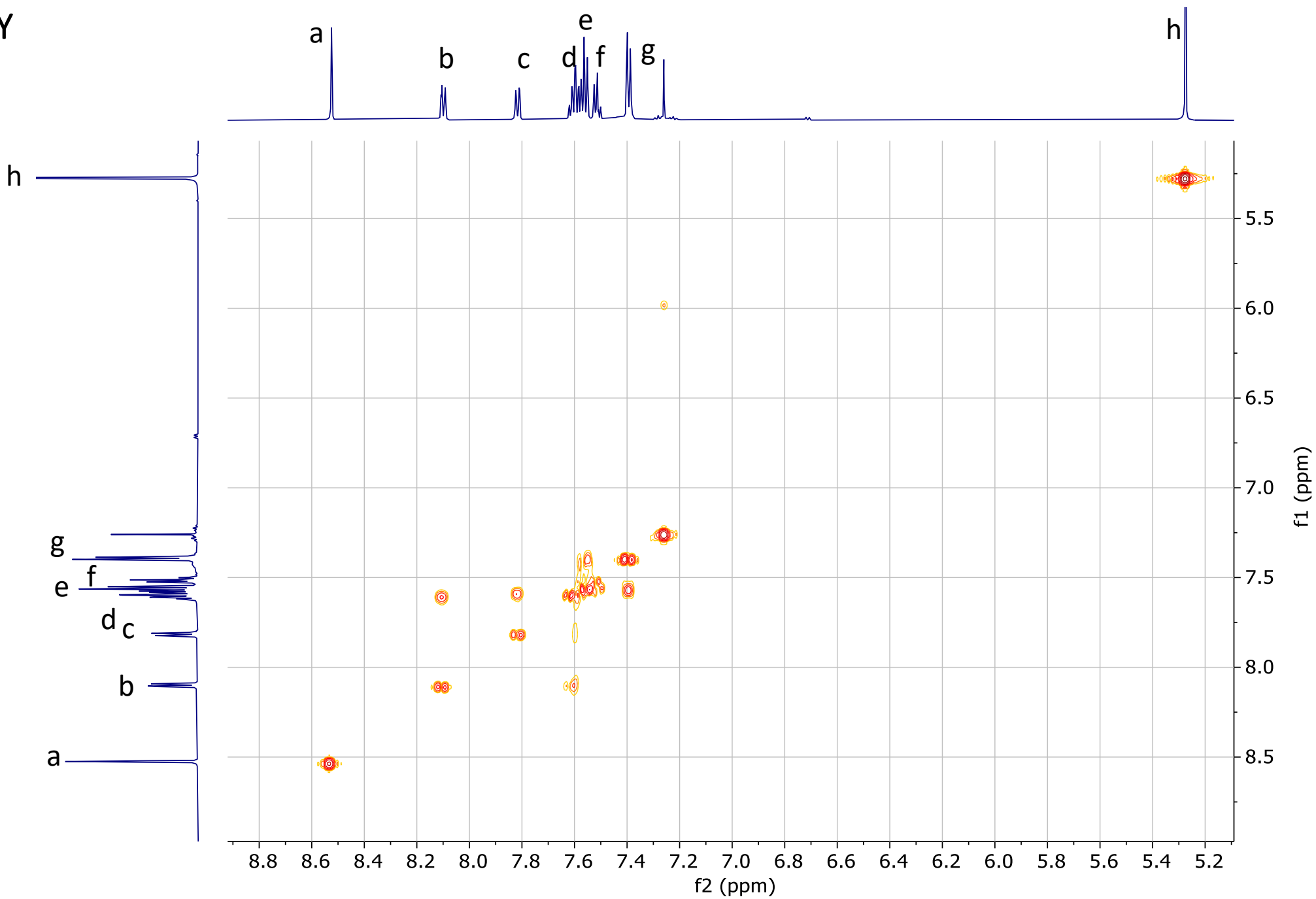
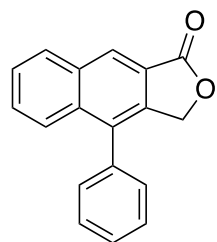
# Type 1- <sup>13</sup>C-NMR Spectrum



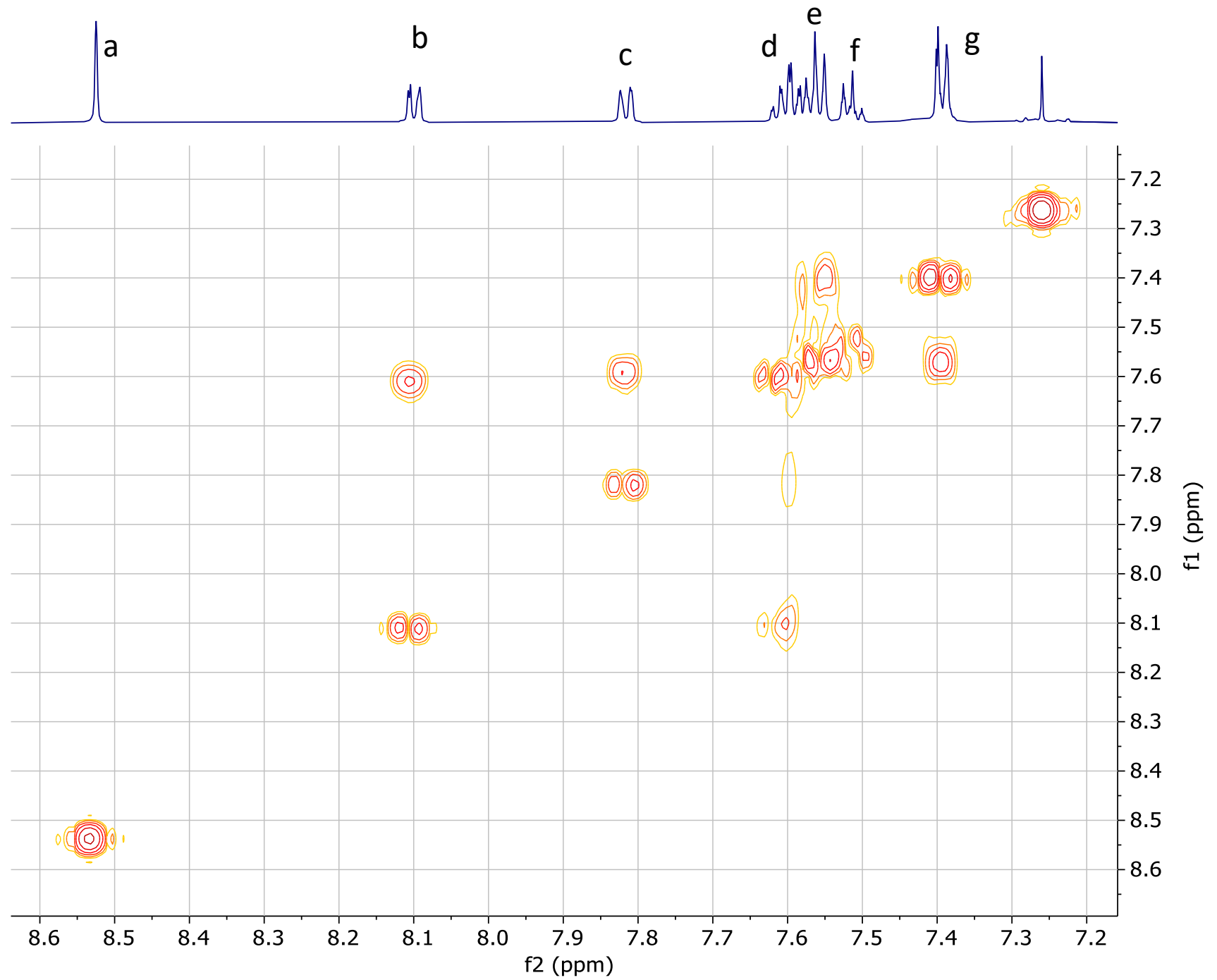
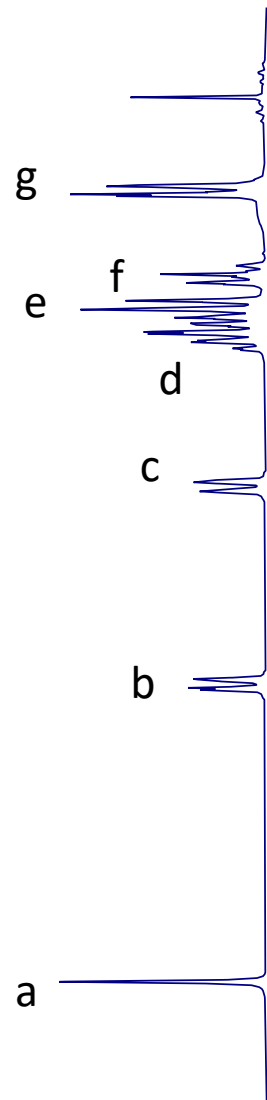
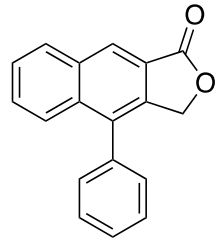
# Type 1 – APT Spectrum



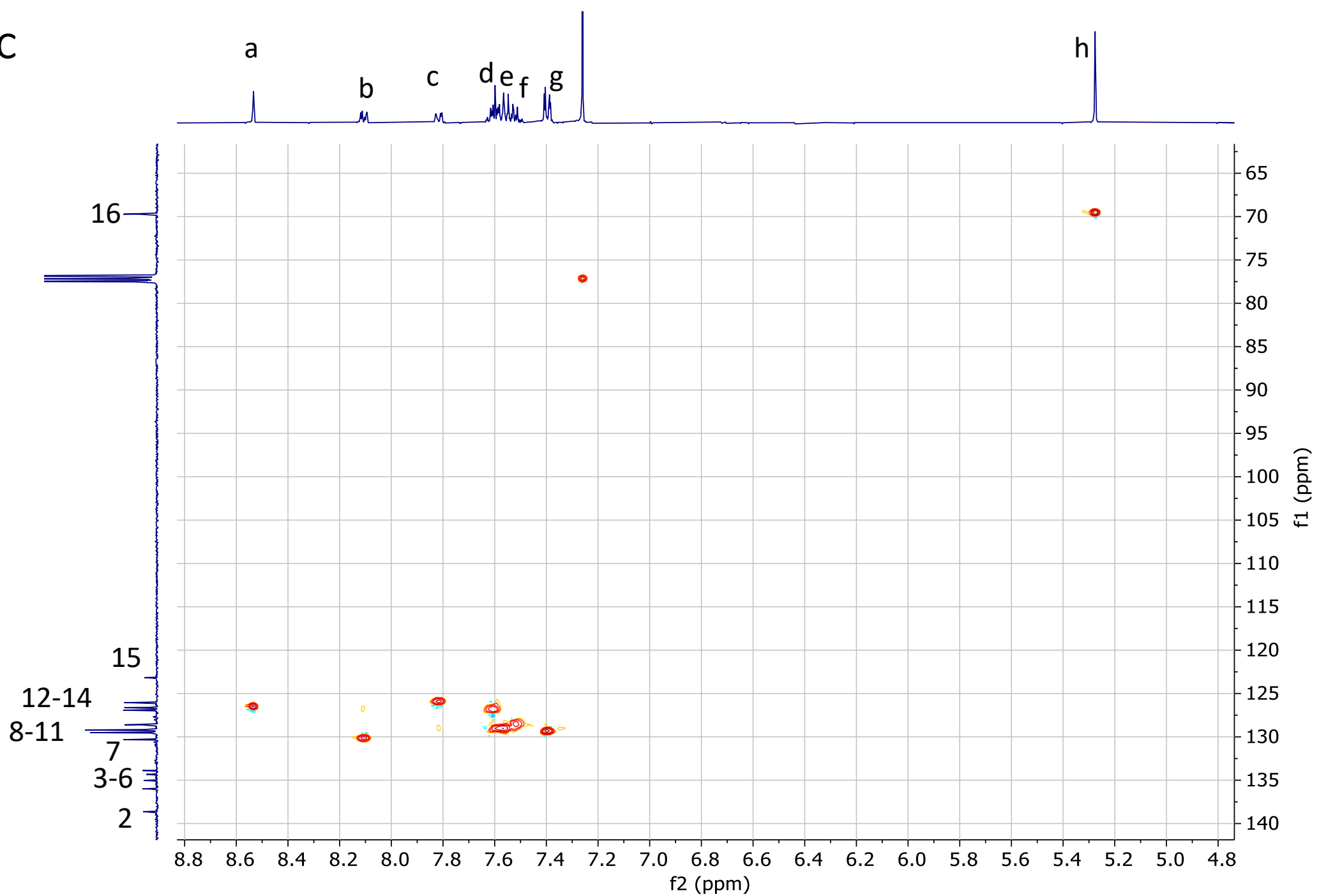
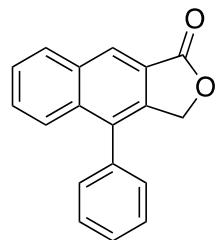
# Type 1 – COSY Spectrum



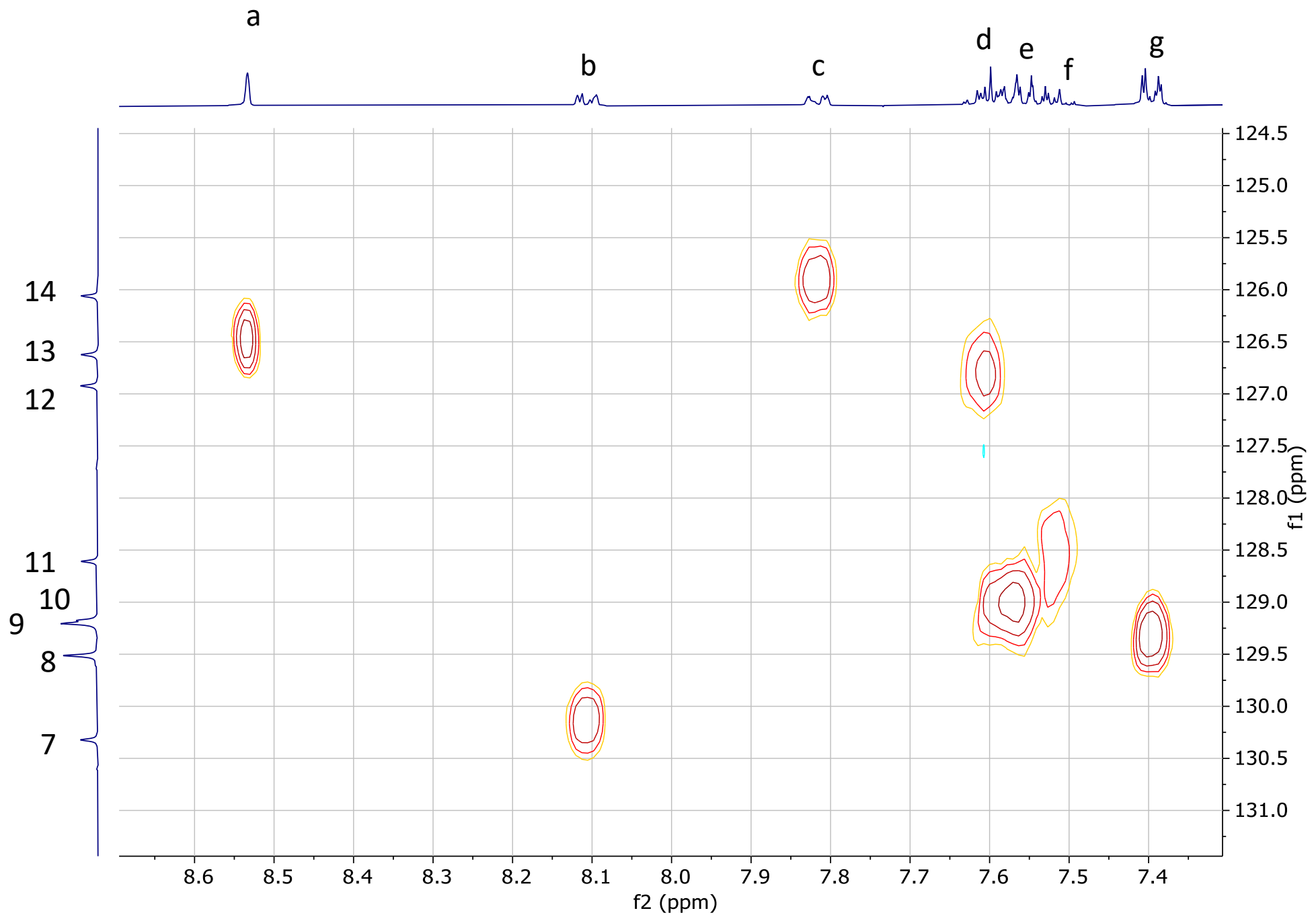
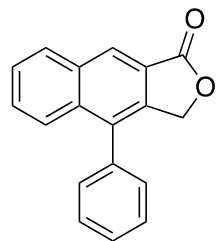
# Type 1 – COSY Spectrum (Zoom)



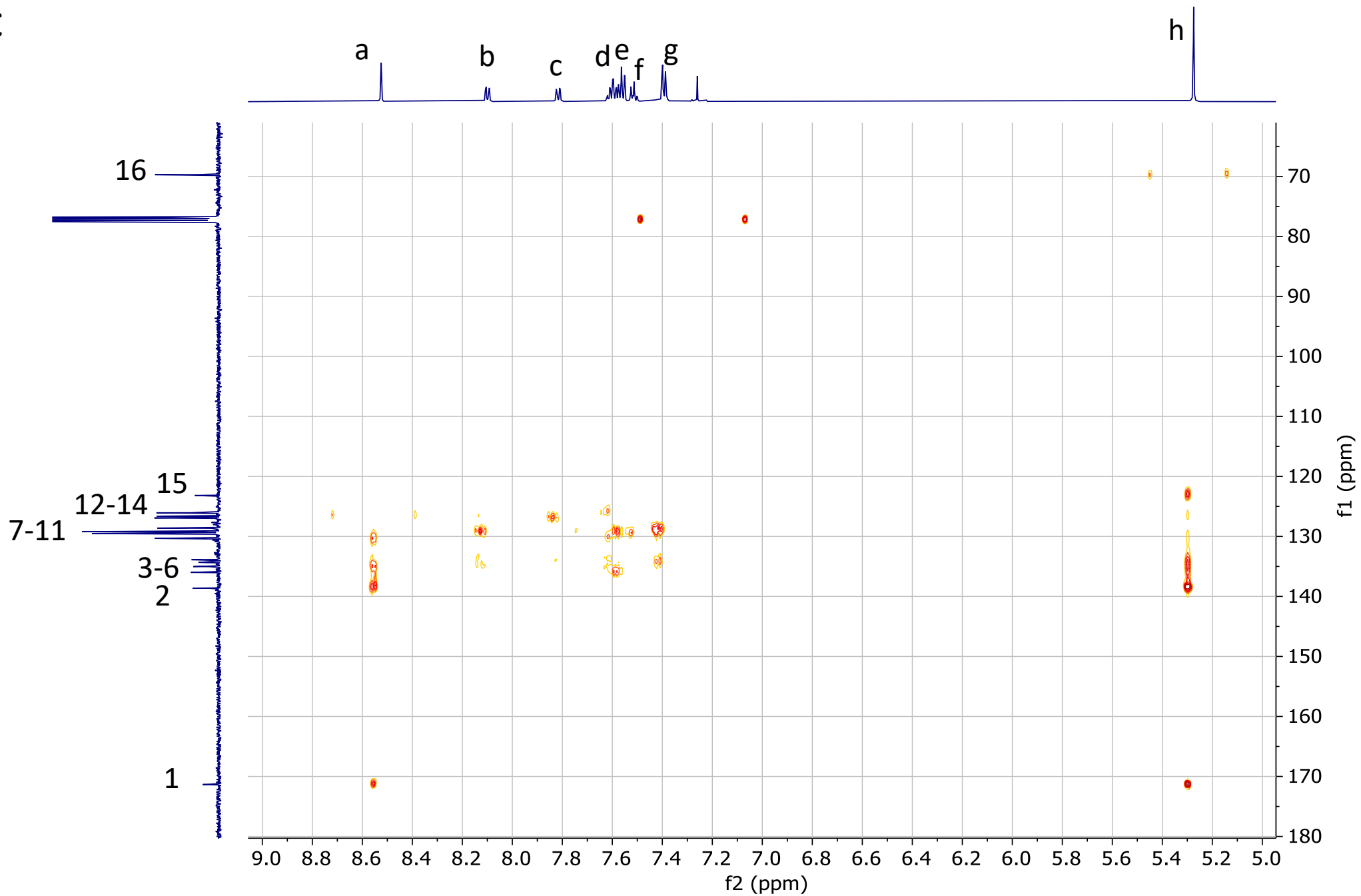
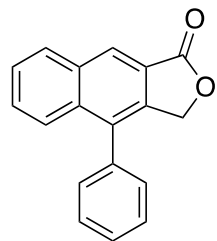
# Type 1 – HSQC Spectrum



# Type 1- HSQC Spectrum (Zoom)

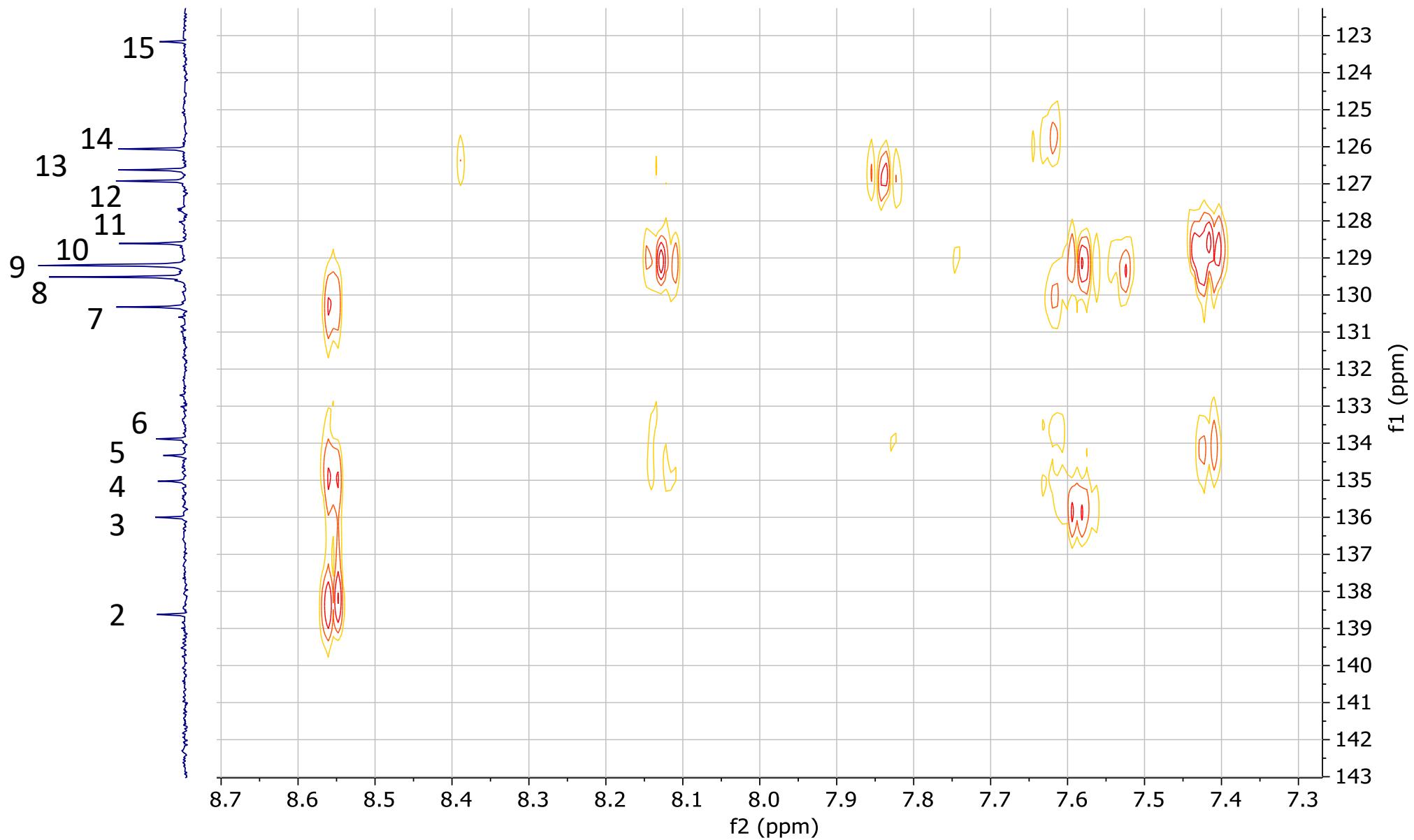
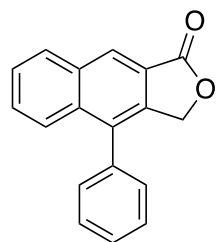


# Type 1- HMBC Spectrum

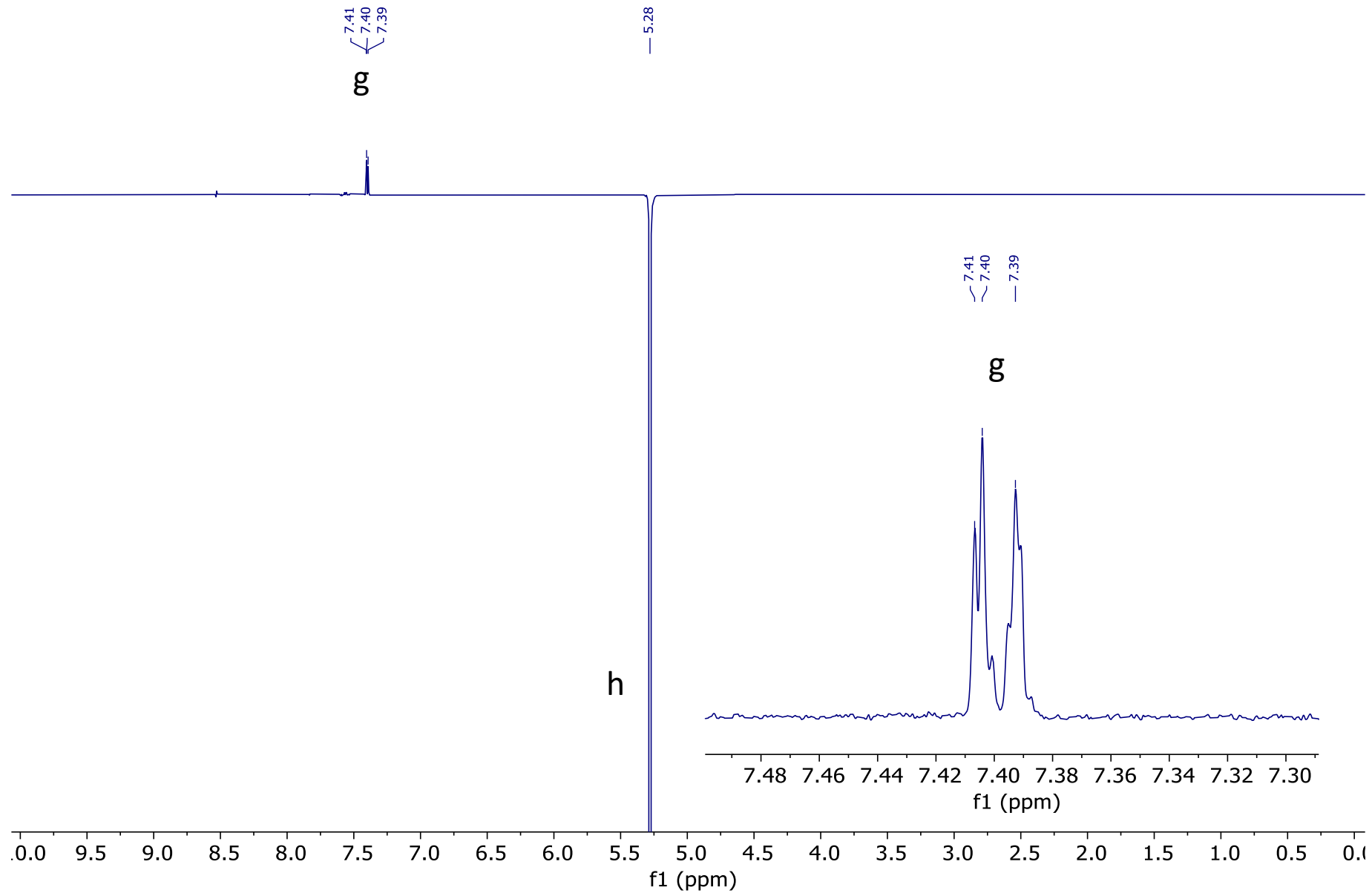
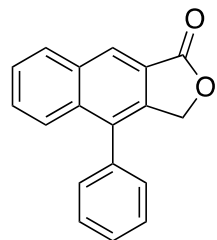




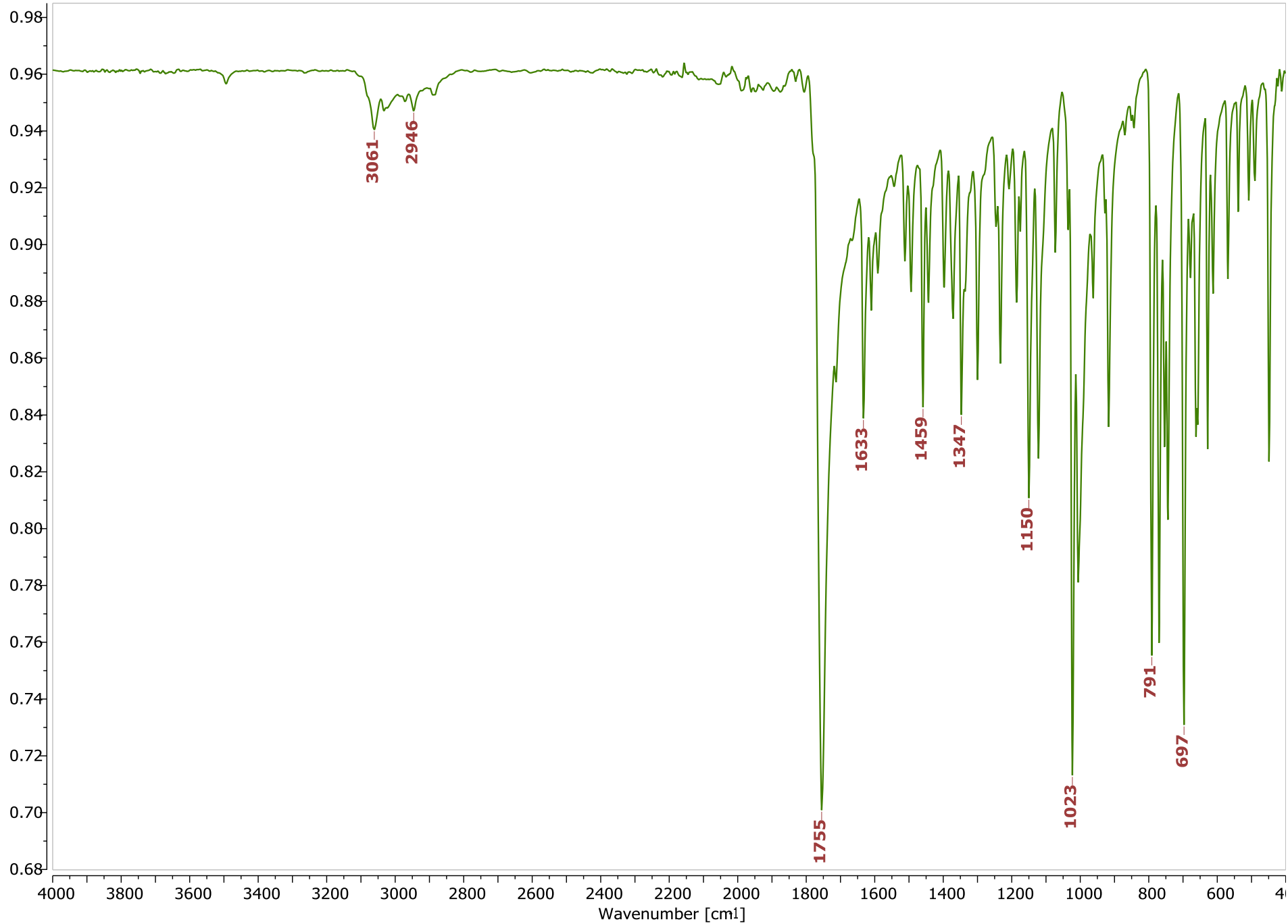
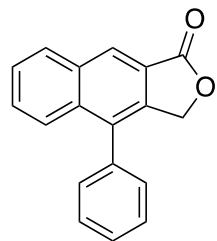
# Type 1- HMBC Spectrum (Zoom)



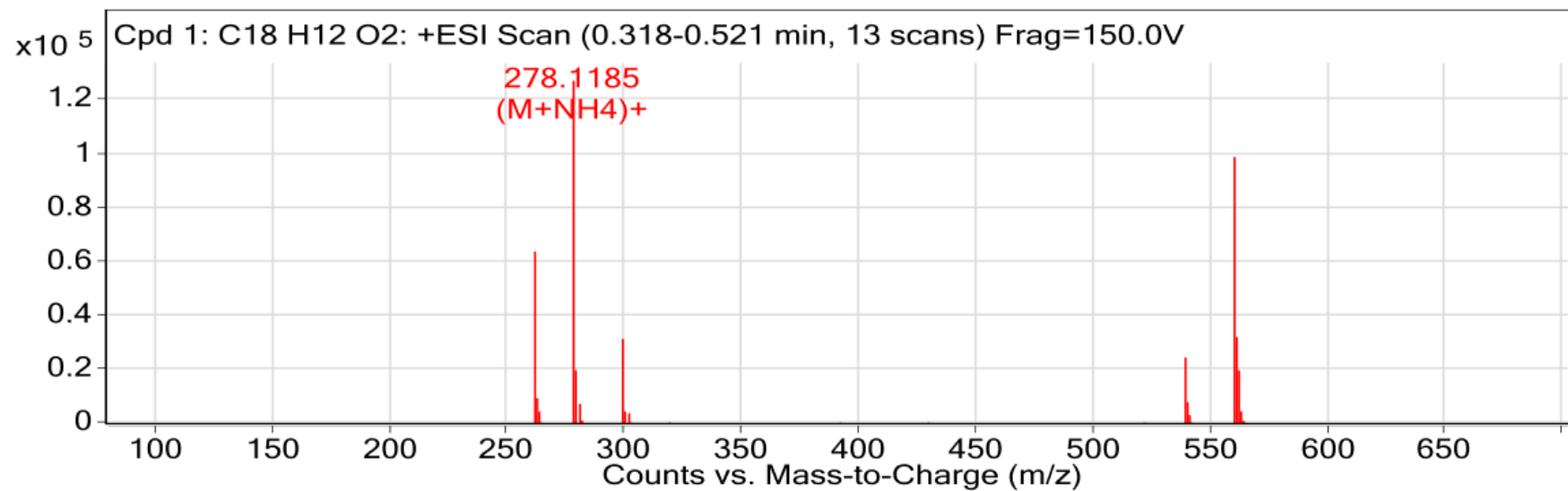
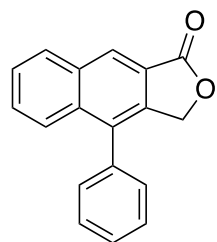
# Type 1- 1D NOE Spectrum



# Type 1 – IR Spectrum

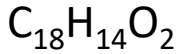


# Type 1 – Mass Spectrum

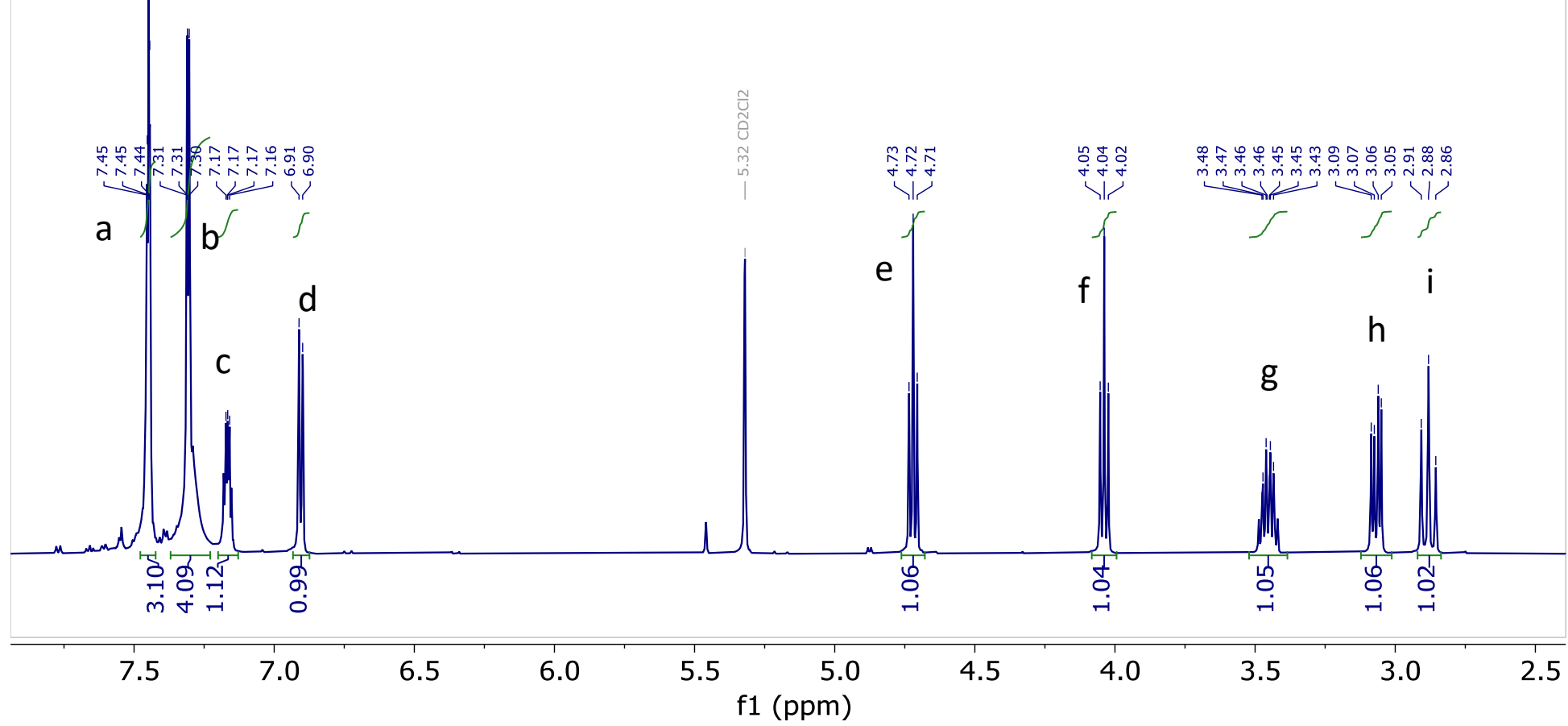
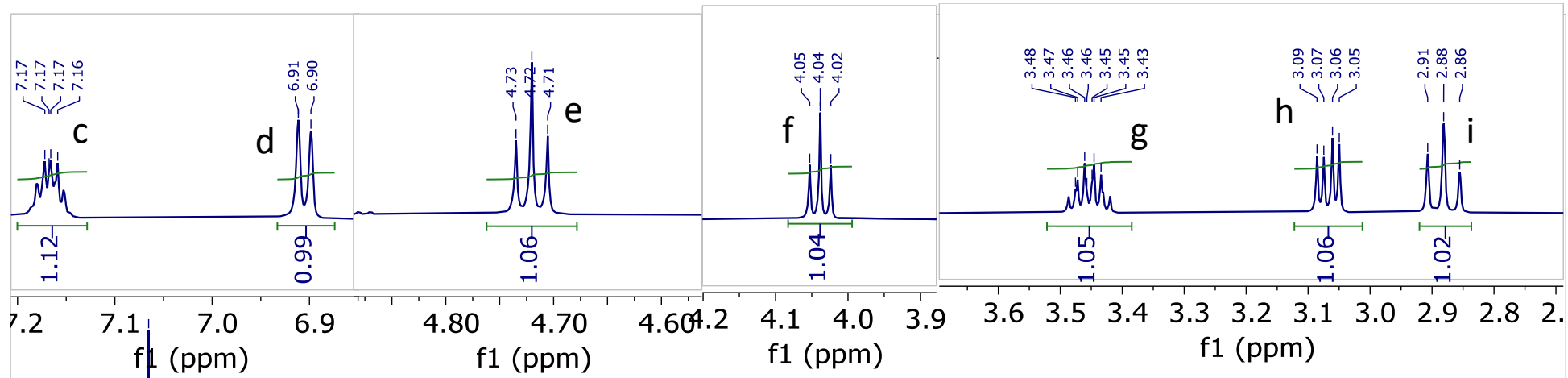


## Peak List

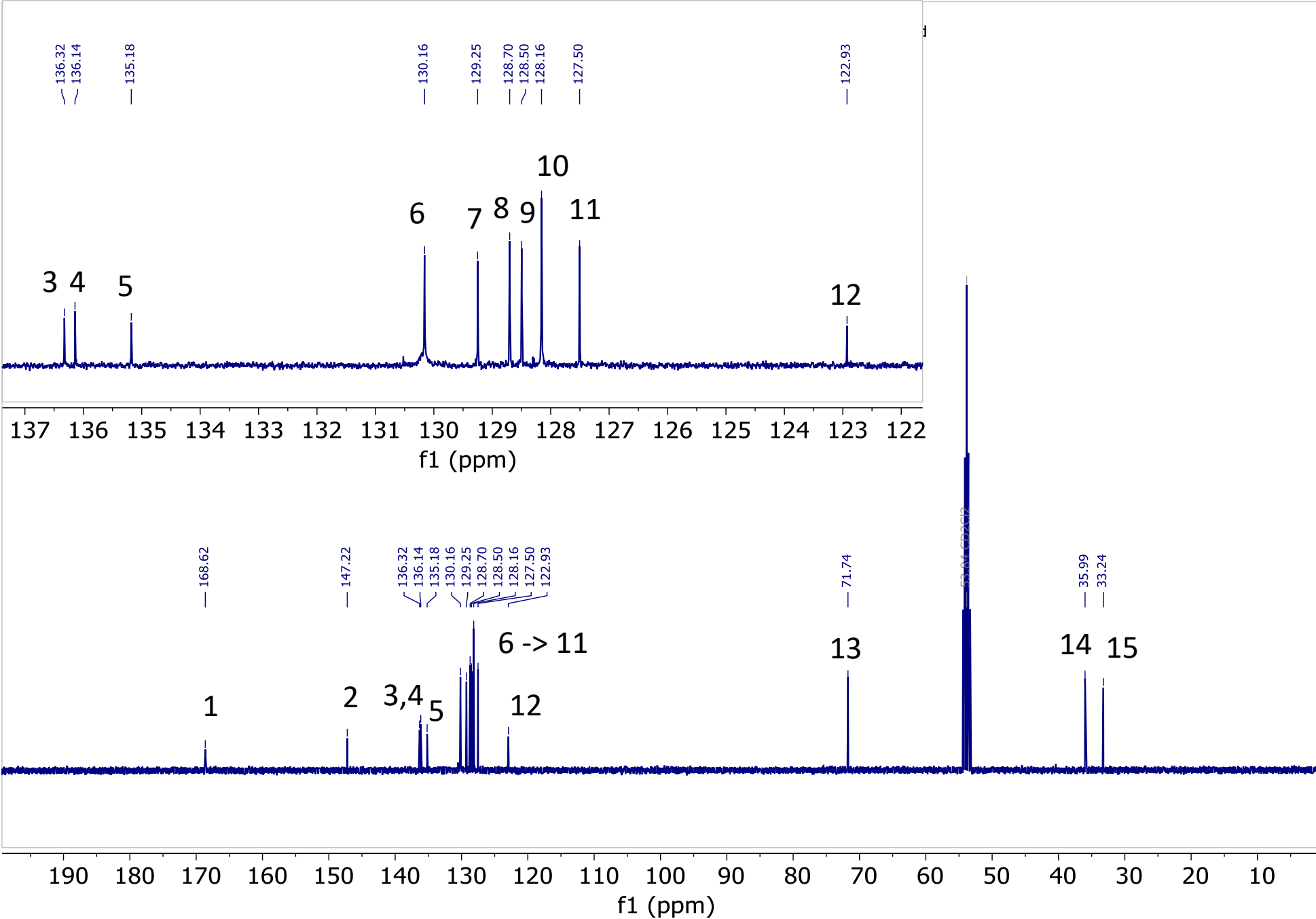
<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
261.0918	1	63705	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
262.0953	1	9659	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
263.1059	1	5072	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
278.1185		127013	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
278.3225		2508		
279.122		19934	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
280.1321		7268	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
299.0481	1	31745	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>
300.051	1	4875	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>
301.0546	1	3806	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>



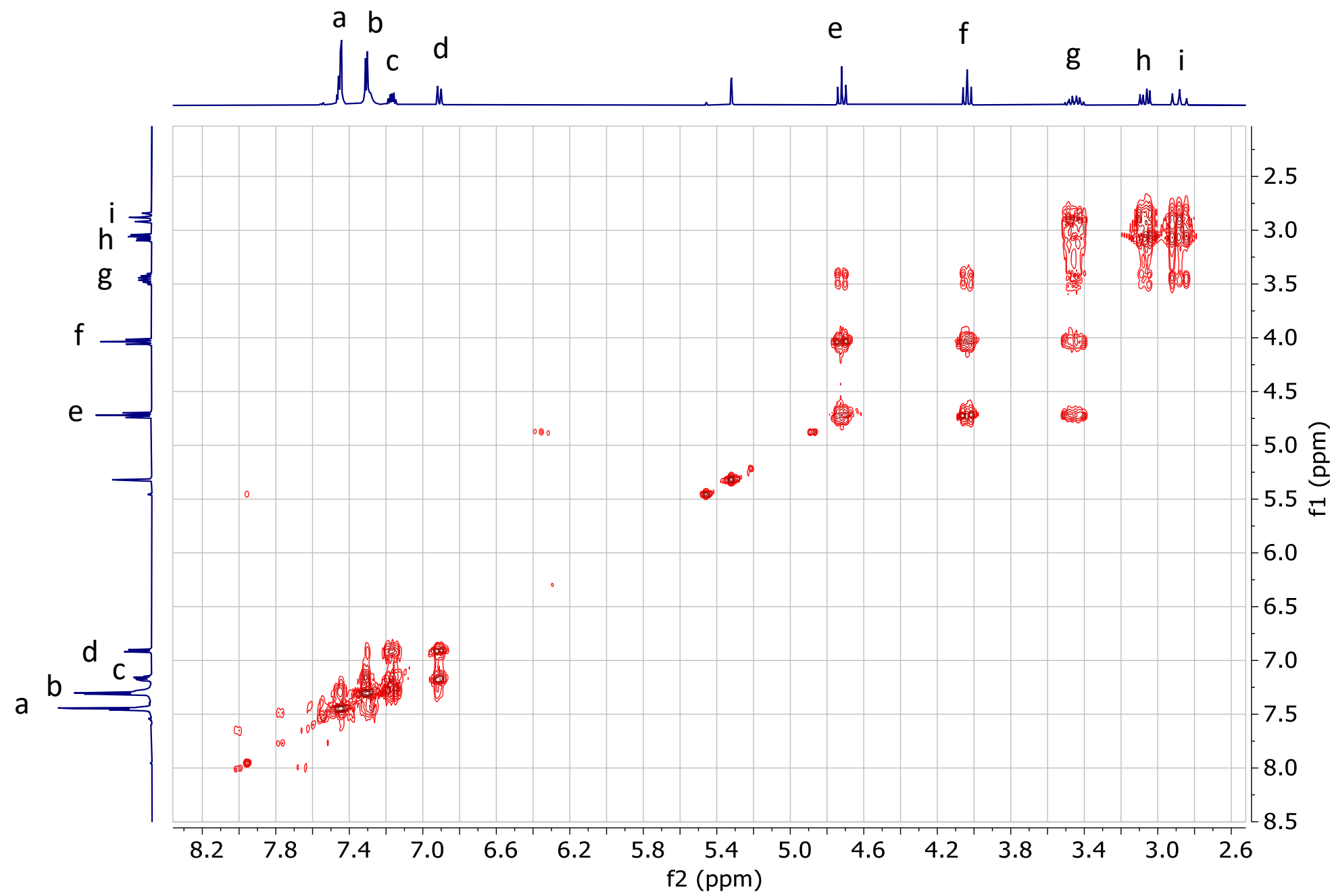
$^1H$  NMR



$C_{18}H_{14}O_2$   
 $^{13}C$  NMR

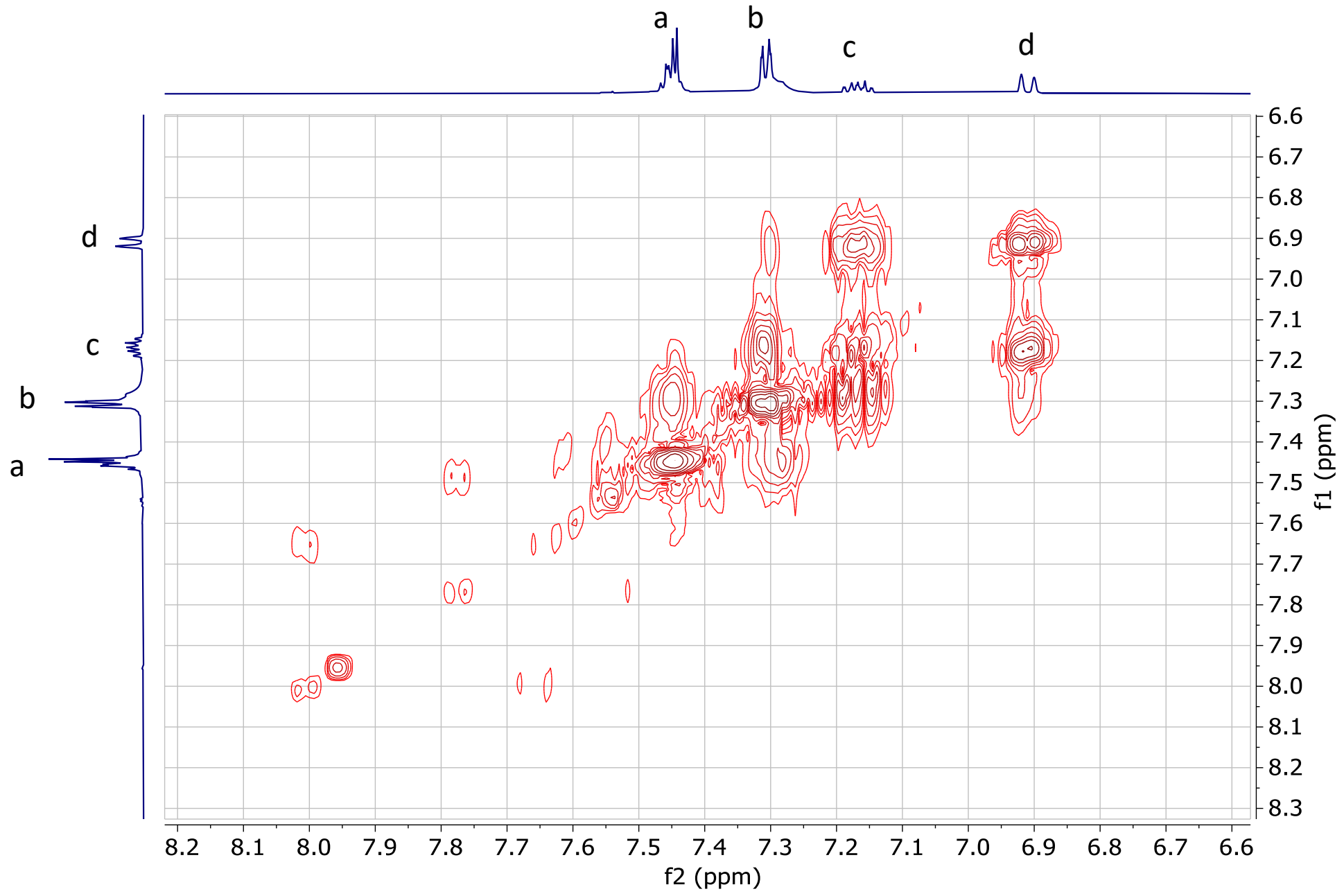


$C_{18}H_{14}O_2$   
COSY



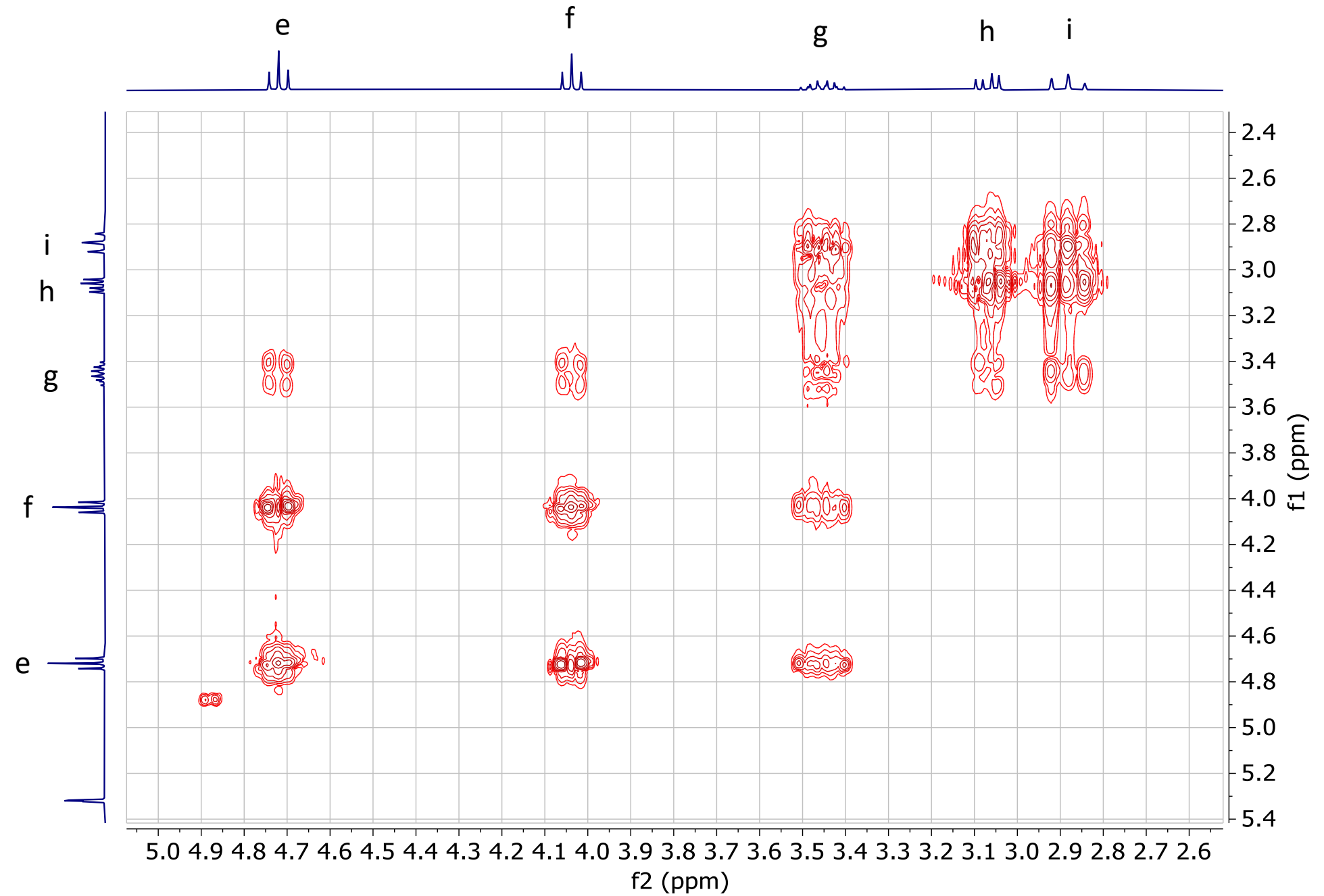
S61

$C_{18}H_{14}O_2$   
COSY (Zoom)



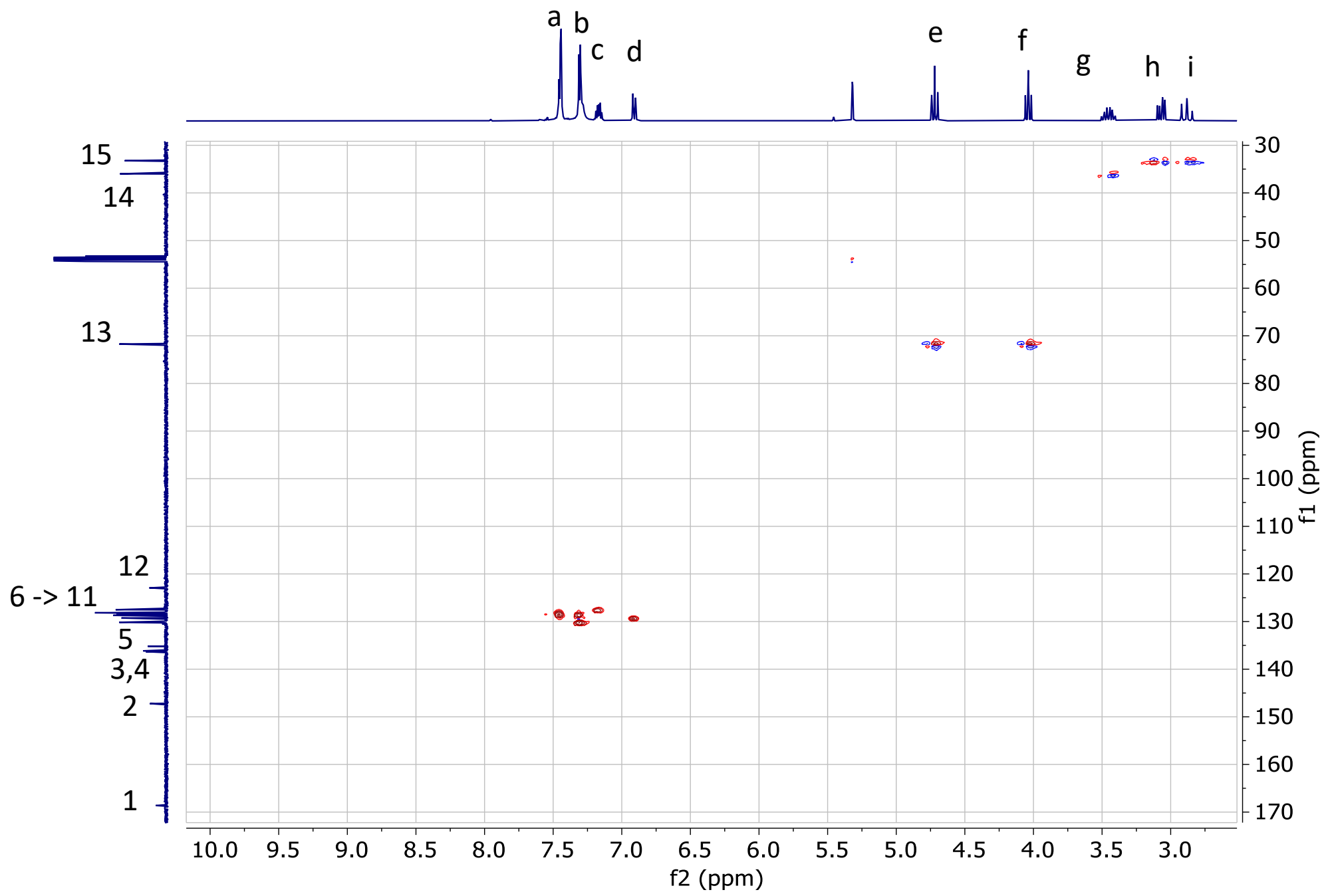


C<sub>18</sub>H<sub>14</sub>O<sub>2</sub>  
COSY (Zoom)

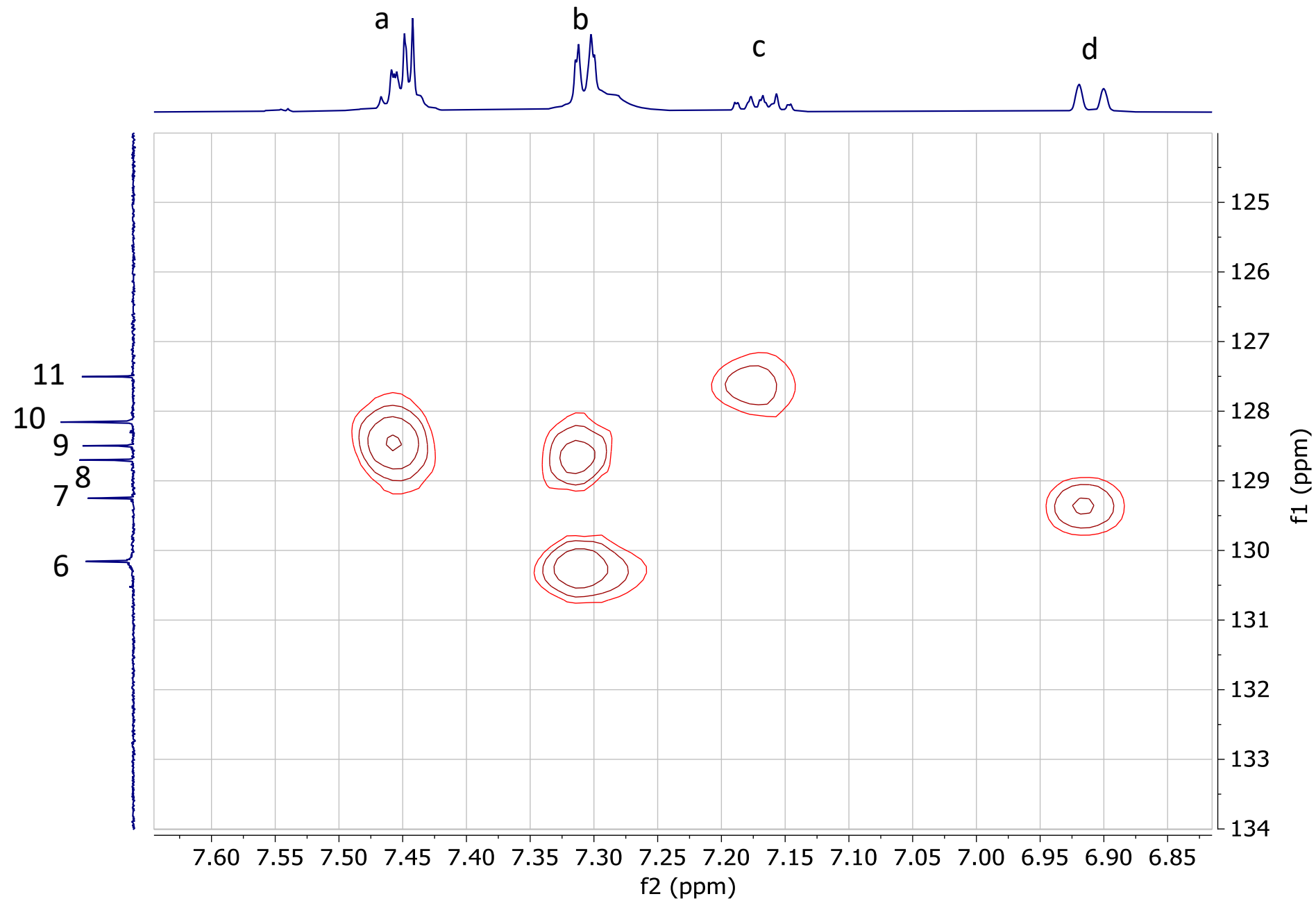


S63

$C_{18}H_{14}O_2$   
HSQC

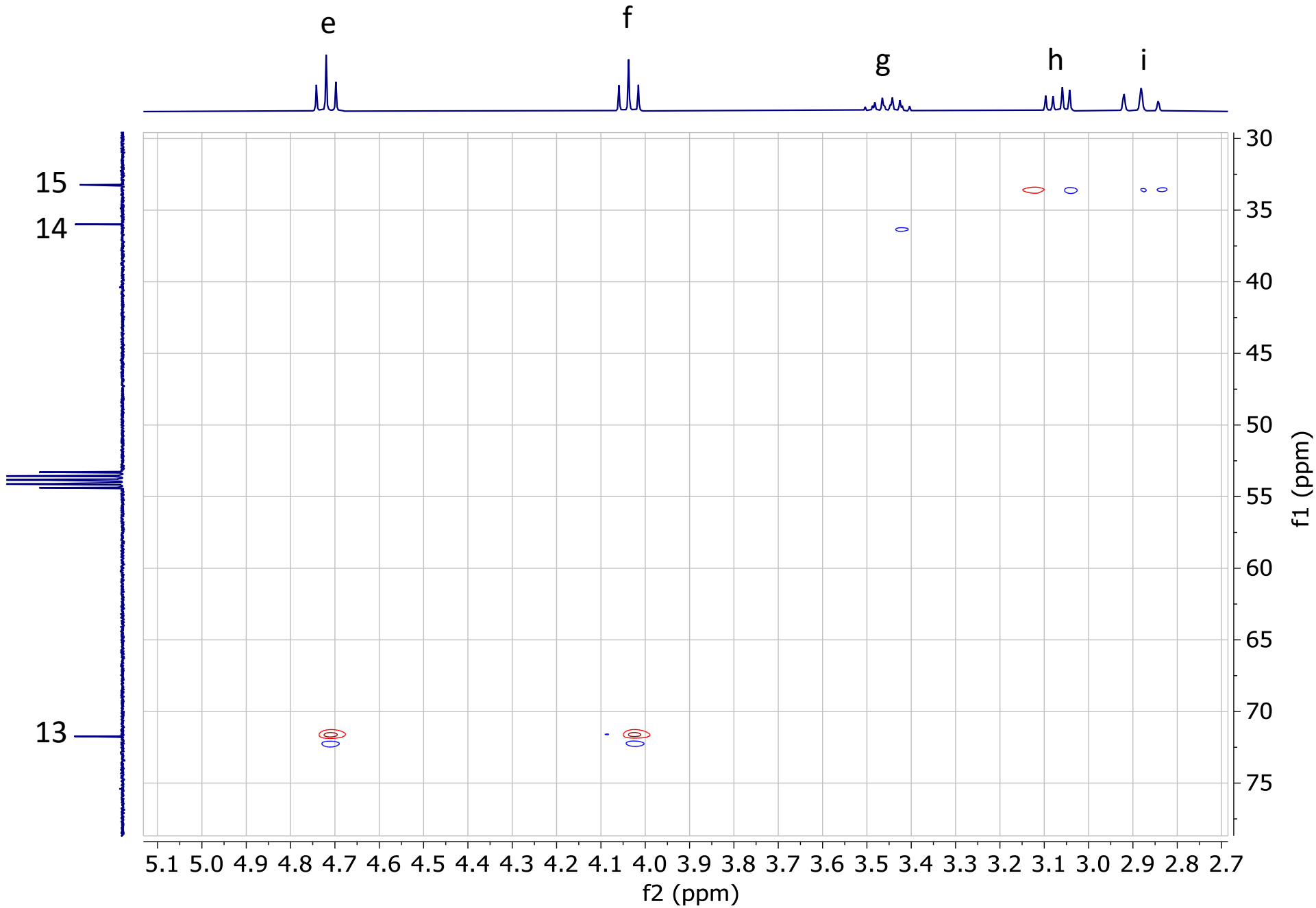


$C_{18}H_{14}O_2$   
HSQC - Zoom

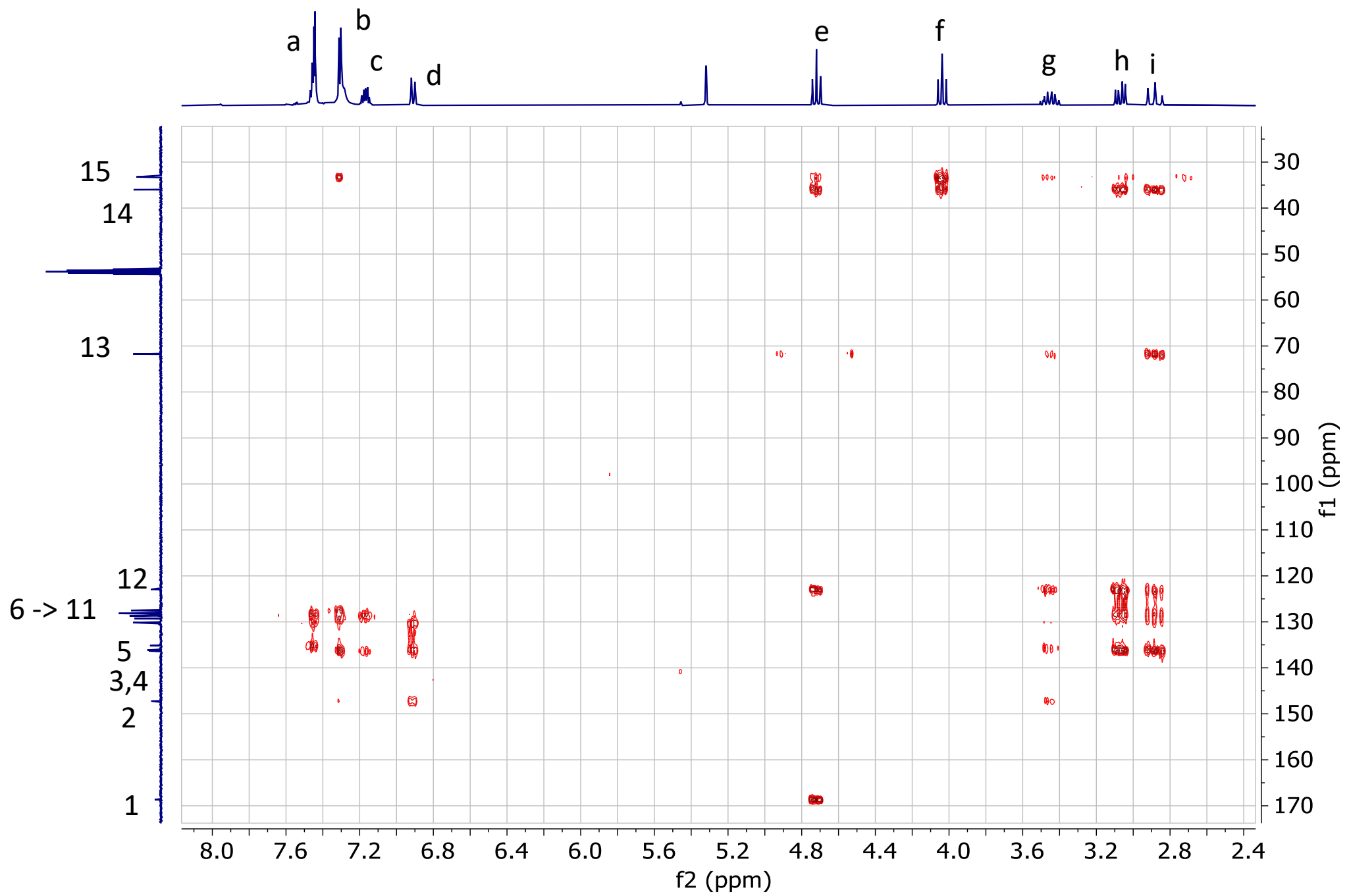


S65

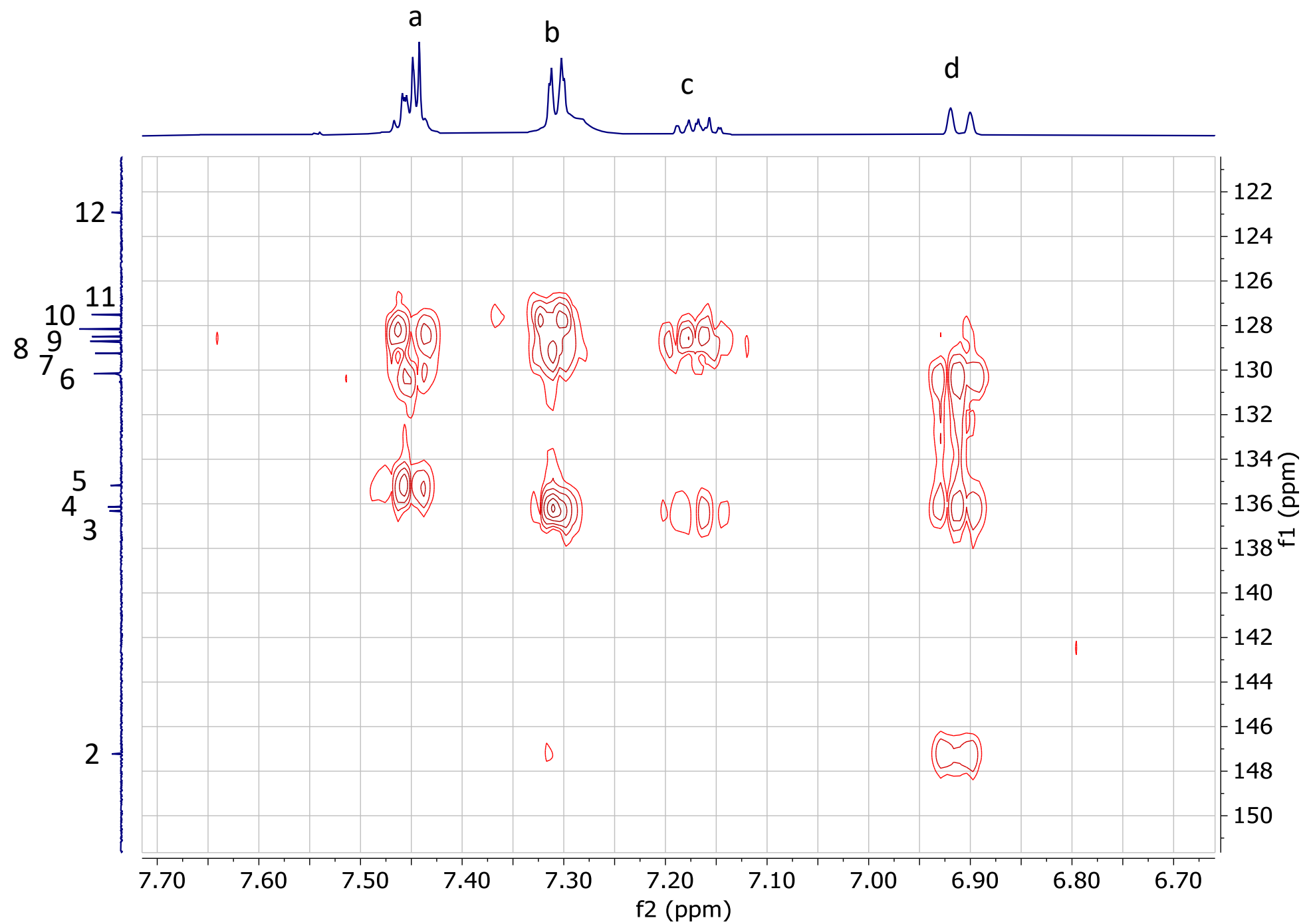
C<sub>18</sub>H<sub>14</sub>O<sub>2</sub>  
HSQC - Zoom



$C_{18}H_{14}O_2$   
HMBC

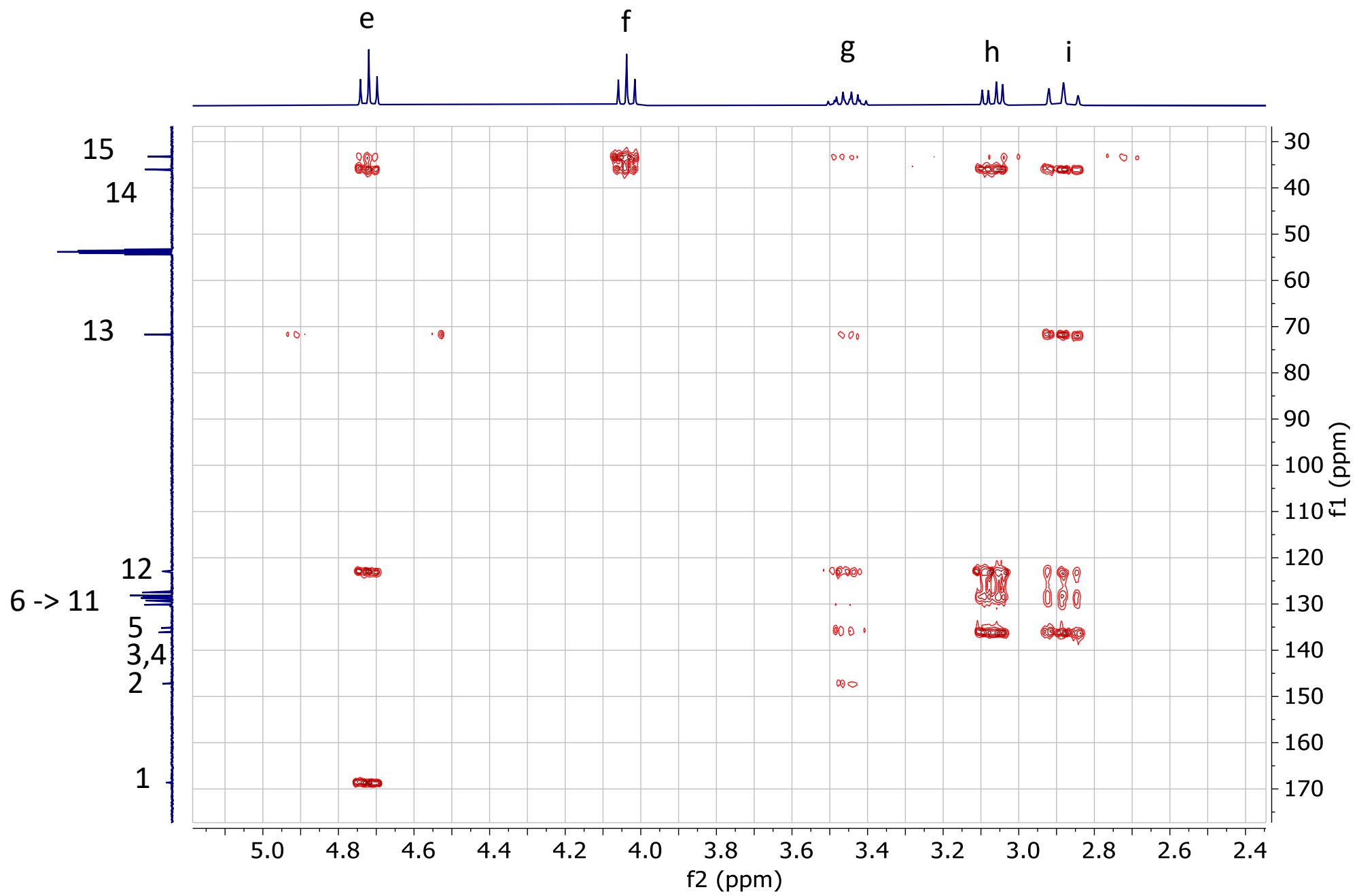


$C_{18}H_{14}O_2$   
HMBC - Zoom

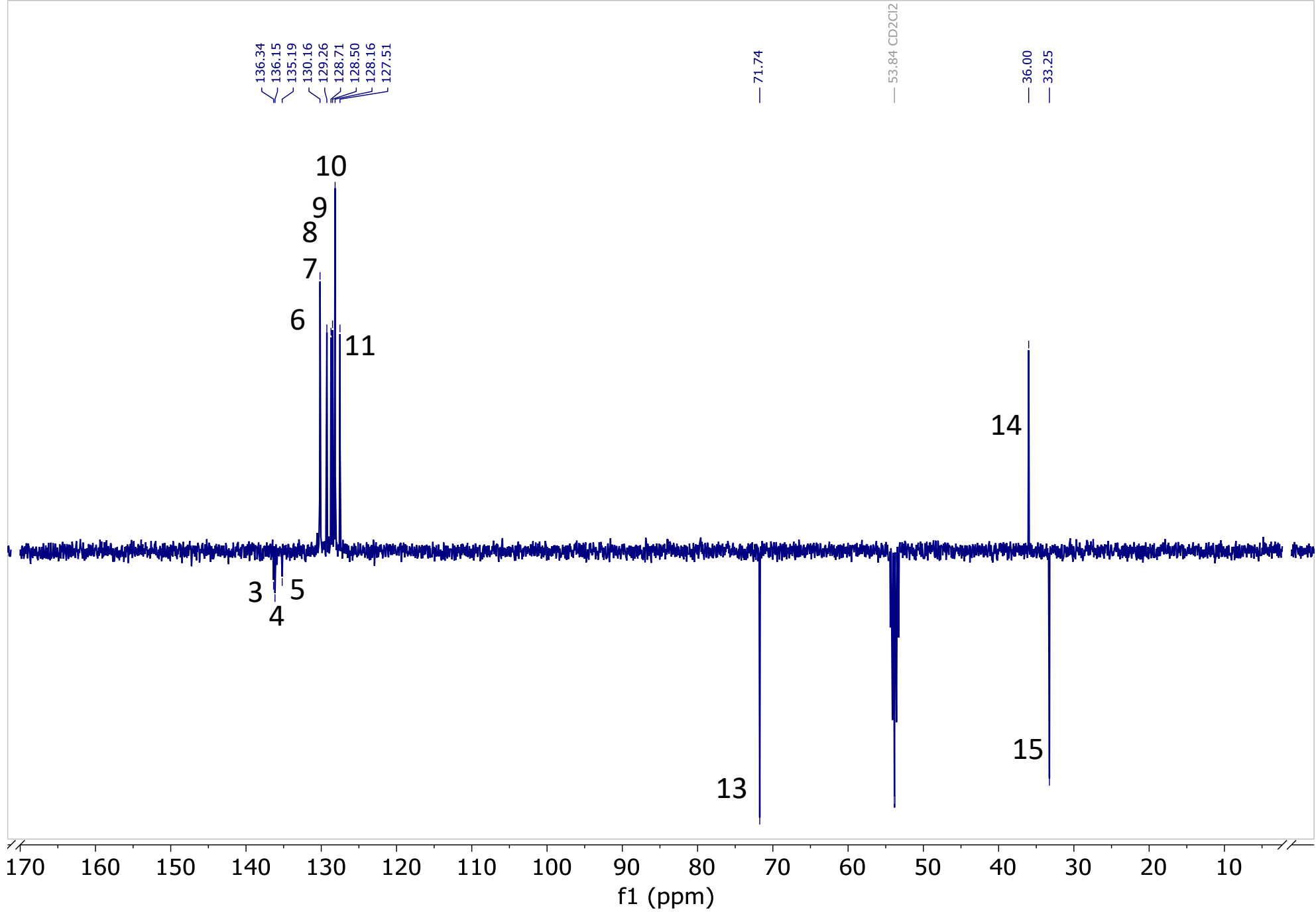


S68

$C_{18}H_{14}O_2$   
HMBC - Zoom

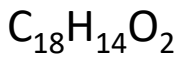


C<sub>18</sub>H<sub>14</sub>O<sub>2</sub>  
DEPT-135

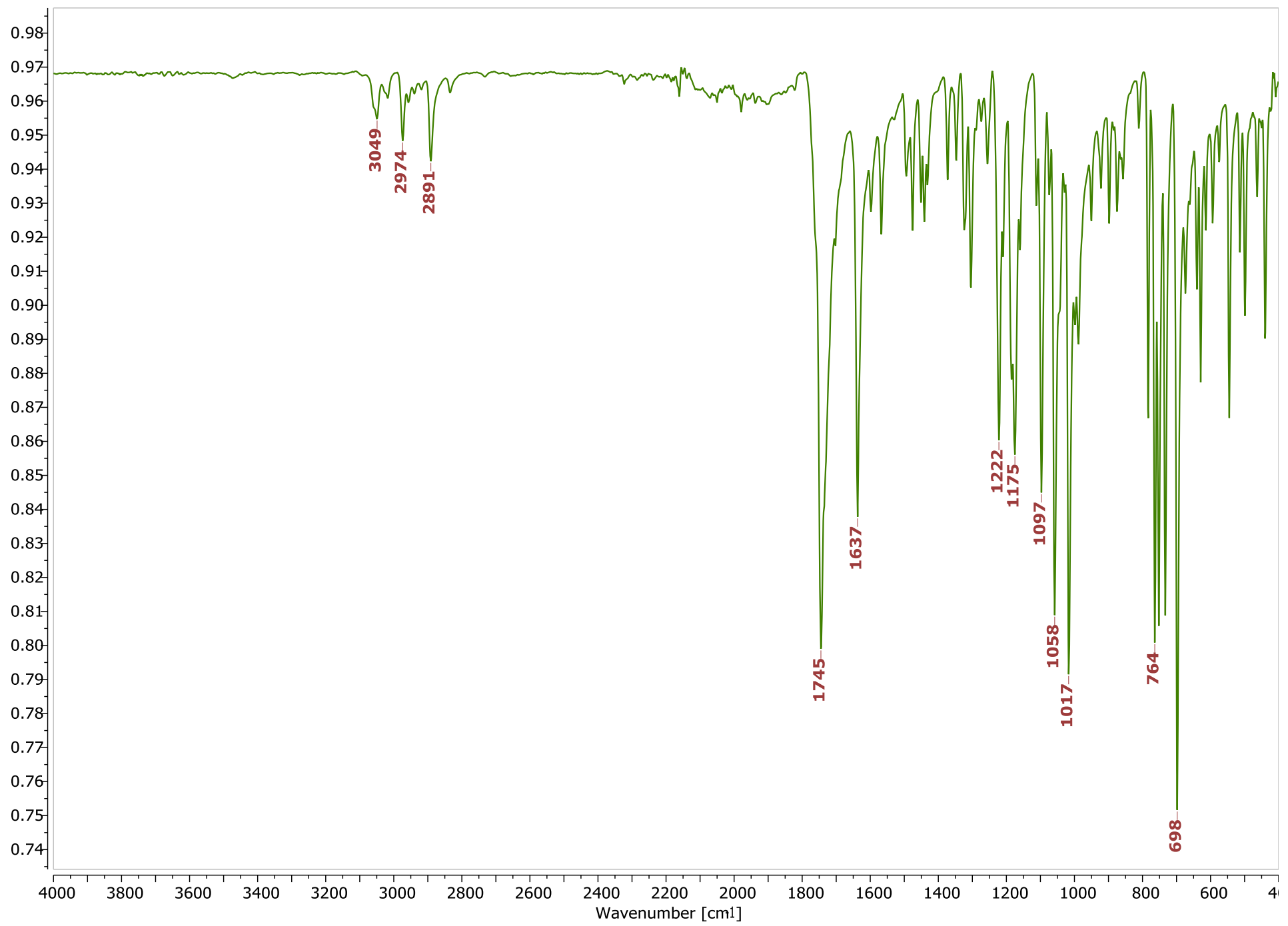


S70



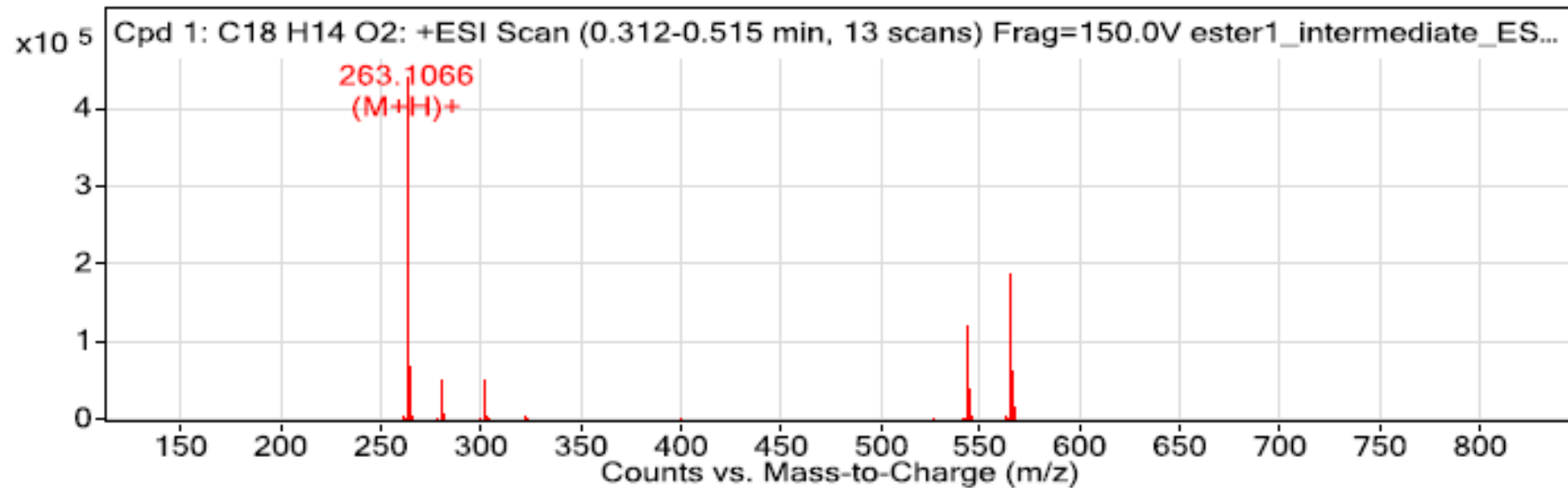


ATR



S71

$C_{18}H_{14}O_2$   
Mass Spectra

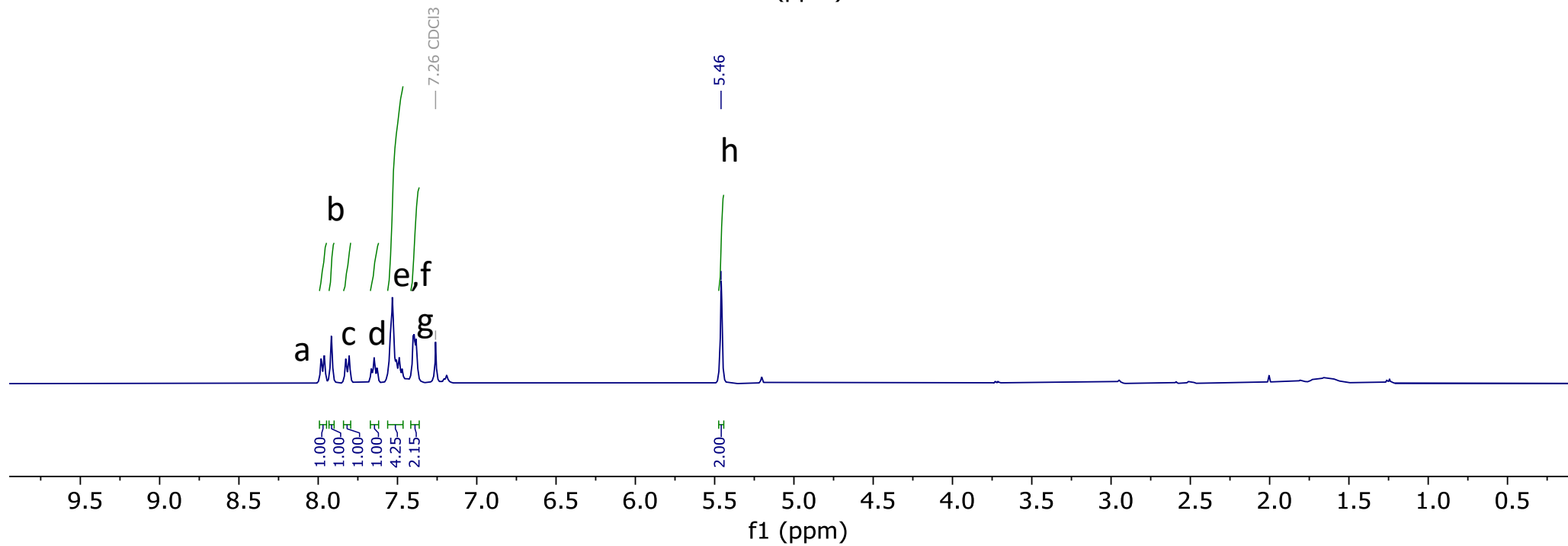
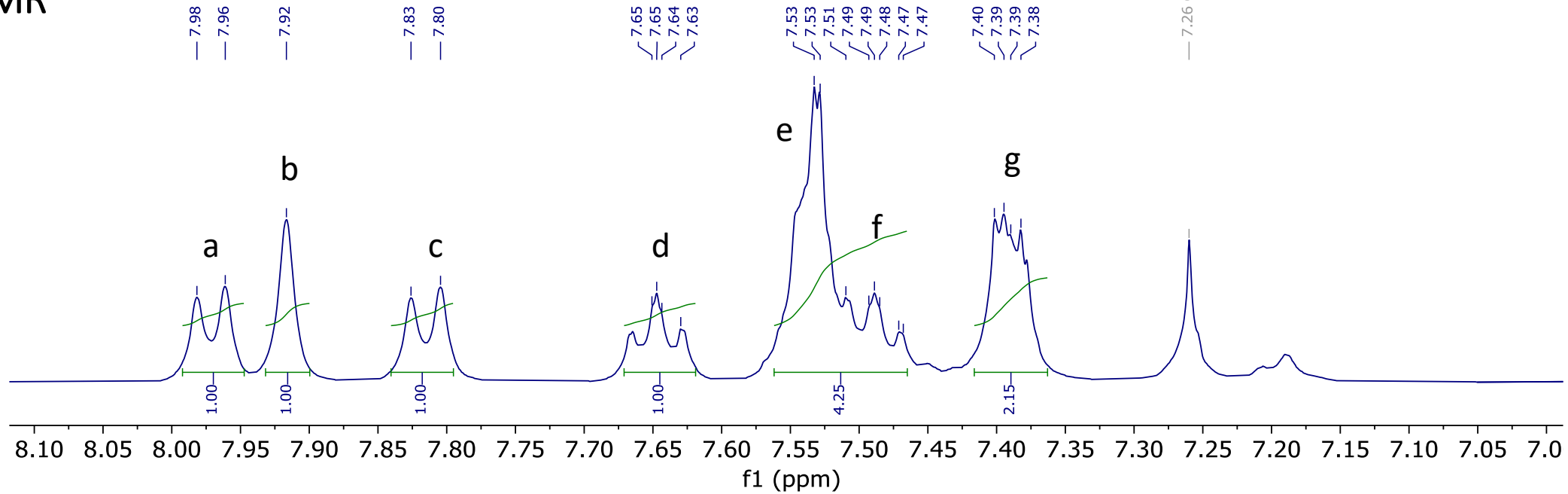
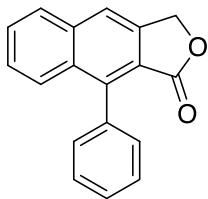


Peak List

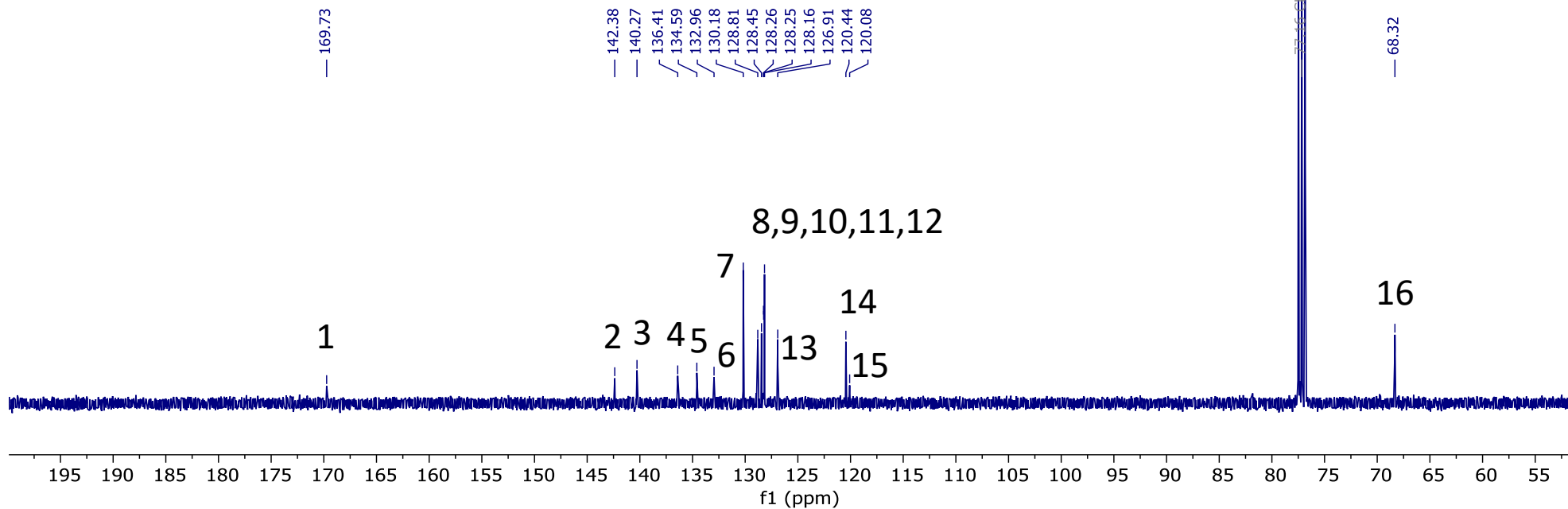
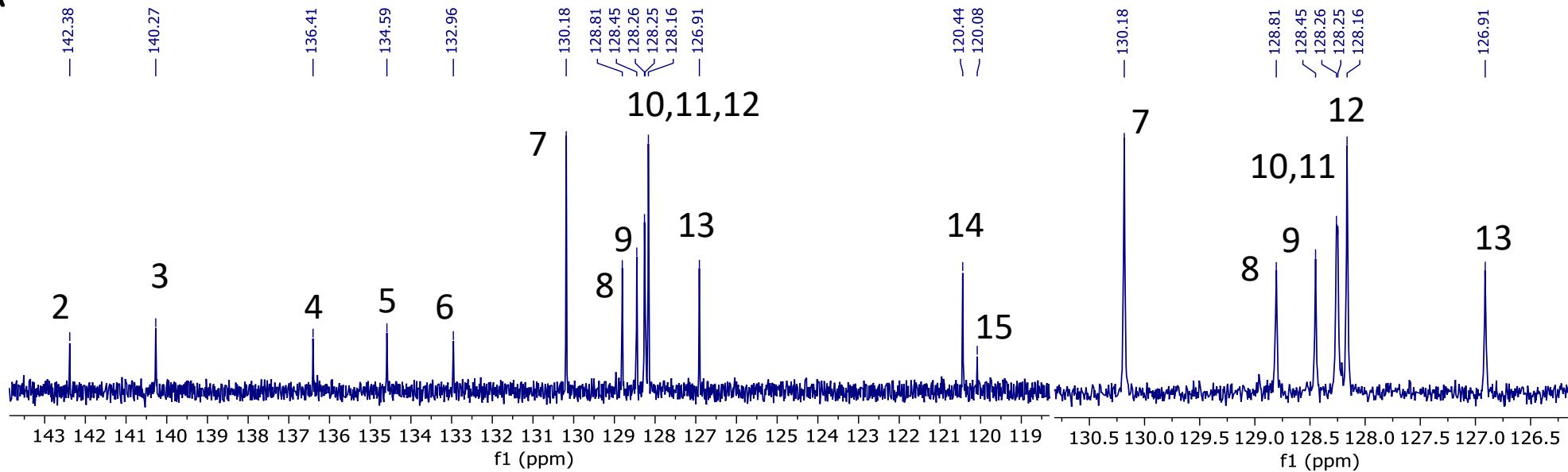
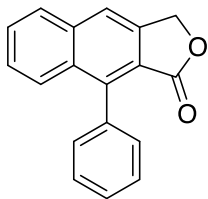
<i>m/z</i>	Abund	Formula	Ion
261.0908	7408		
262.0947	1389		
263.1066	441115	C18 H15 O2	(M+H)+
263.3059	24011		
263.4134	1213		
263.5078	1653		
263.7091	711		
264.1098	71591	C18 H15 O2	(M+H)+
264.3112	1443		
265.1127	6262	C18 H15 O2	(M+H)+

--- End Of Report ---

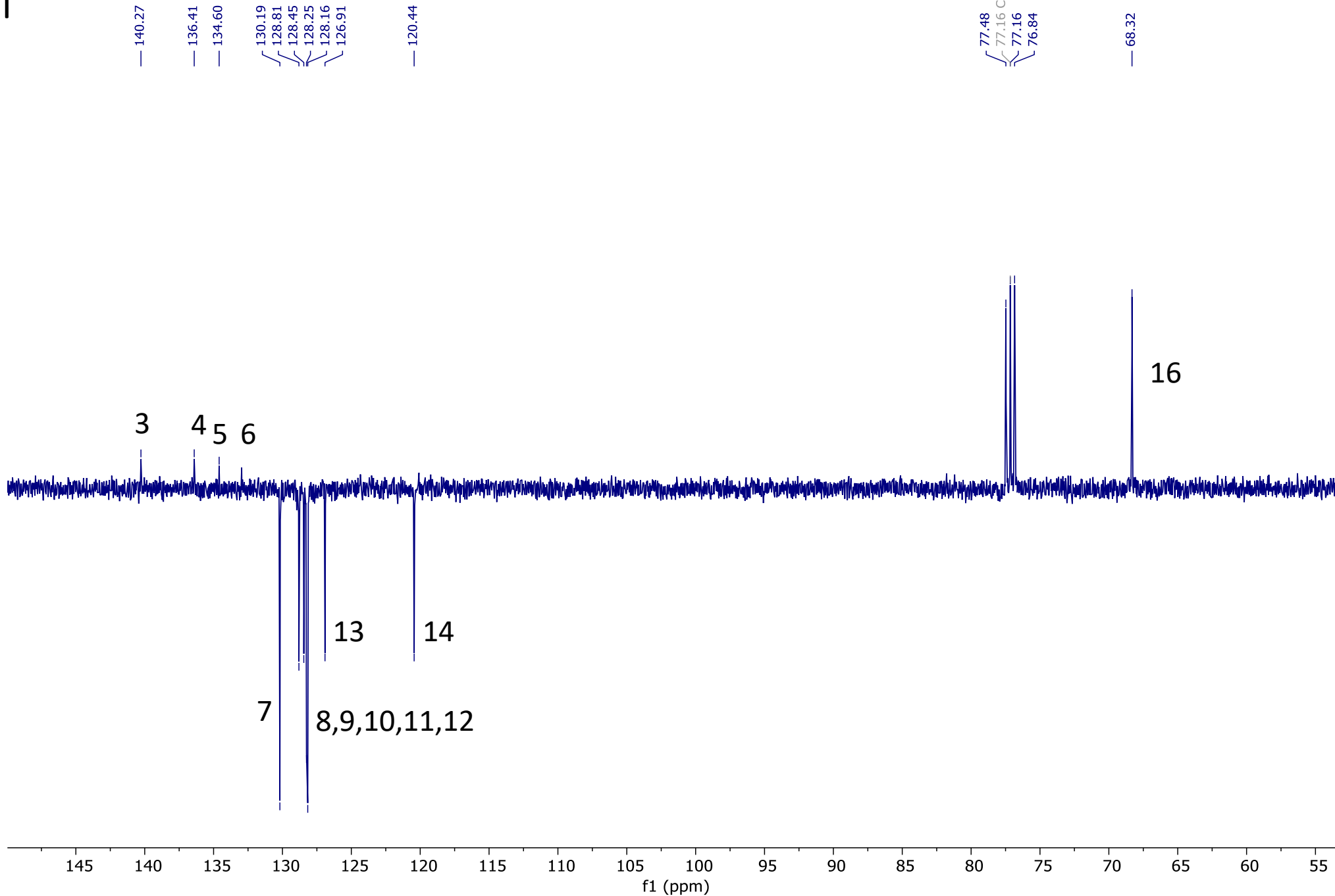
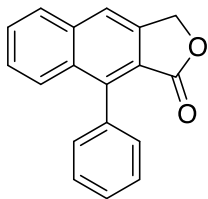
# Type 2 – <sup>1</sup>H-NMR Spectrum



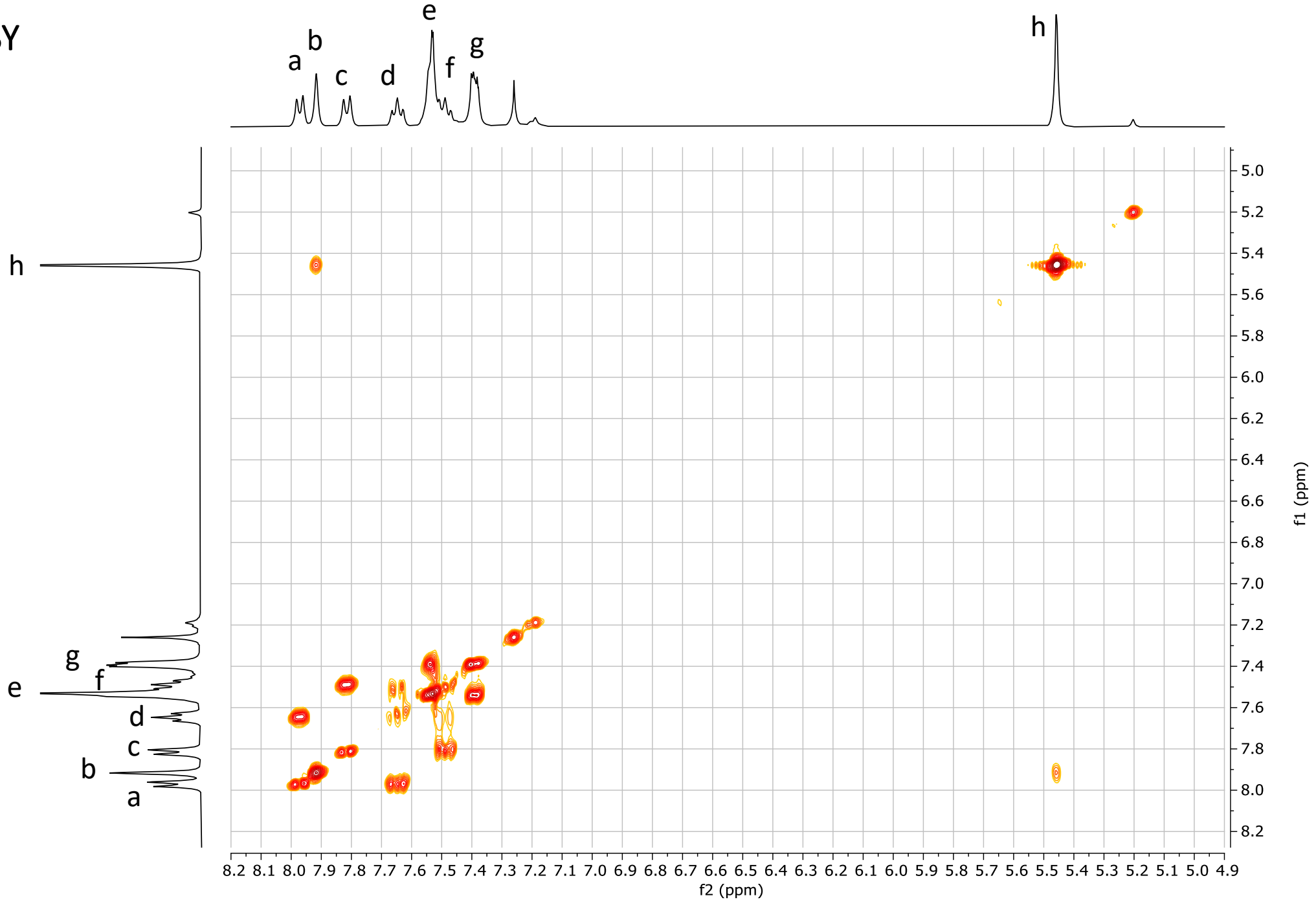
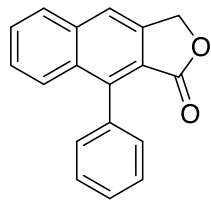
# Type 2 – <sup>13</sup>C-NMR Spectrum



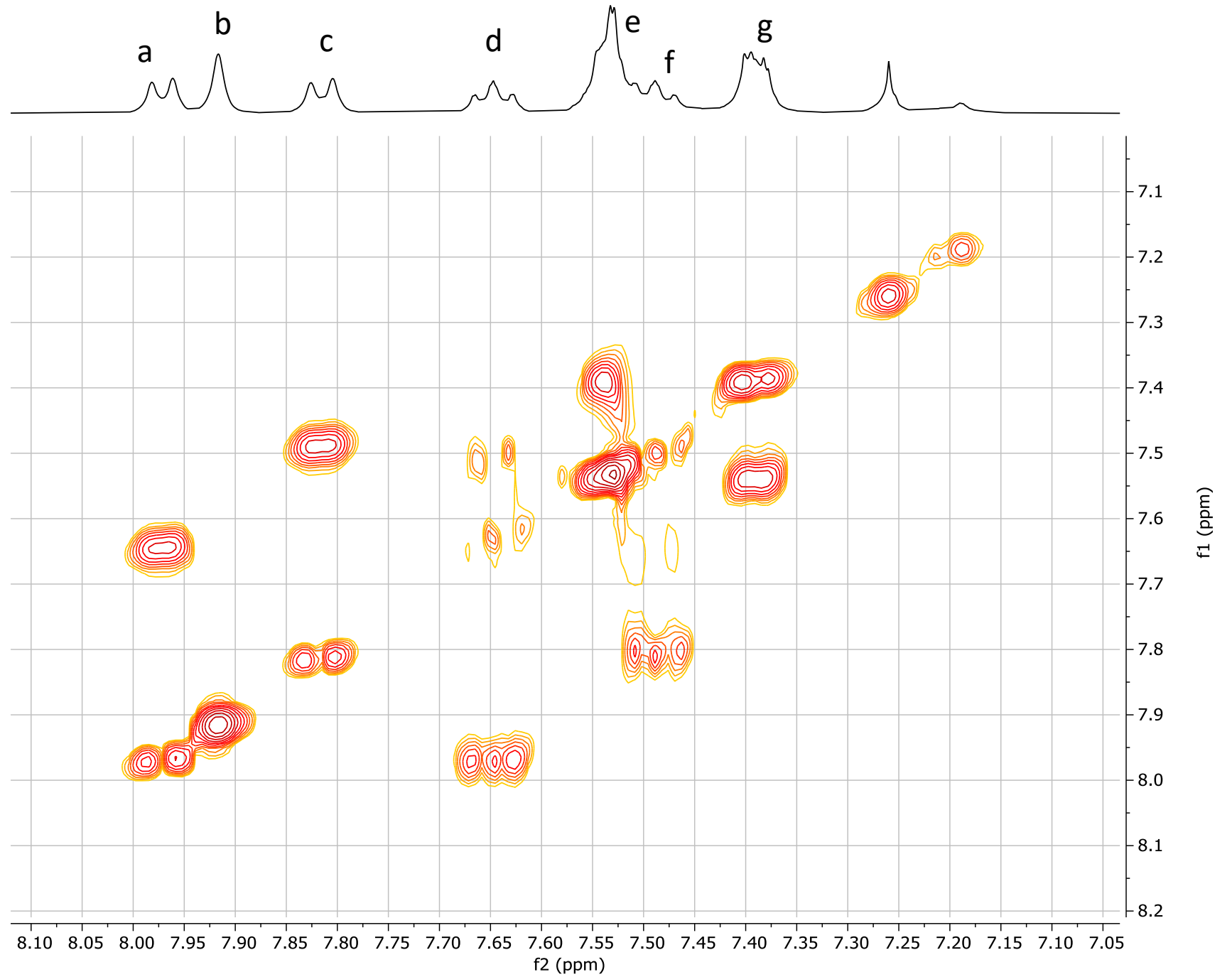
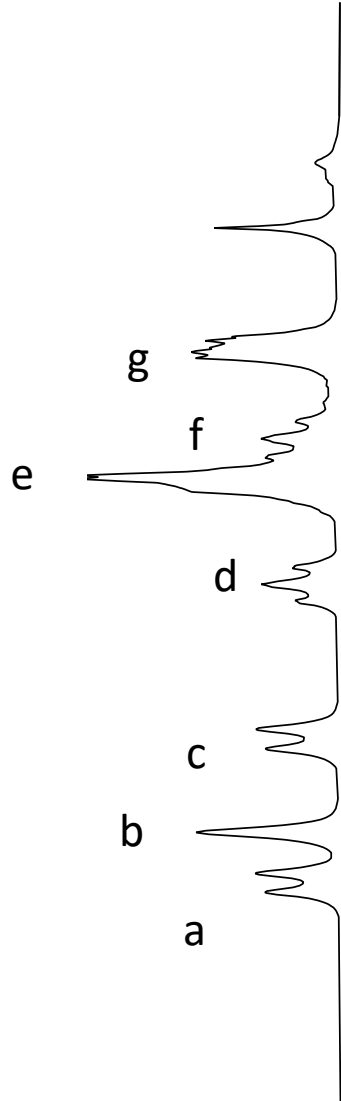
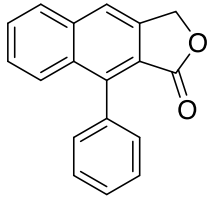
# Type 2 – APT Spectrum



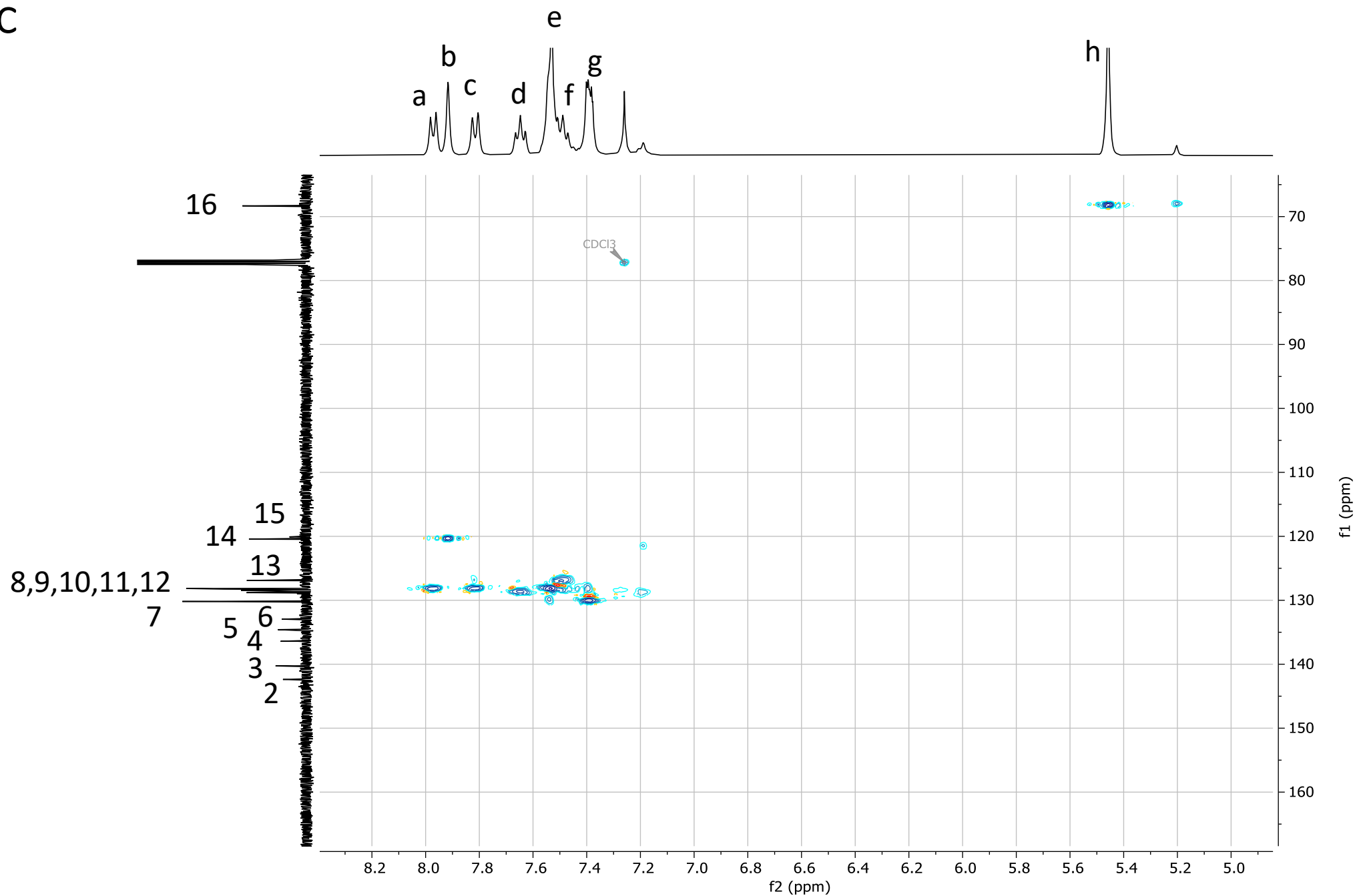
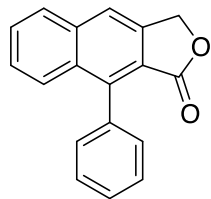
# Type 2 – COSY Spectrum



# Type 2 – COSY Spectrum (Zoom)

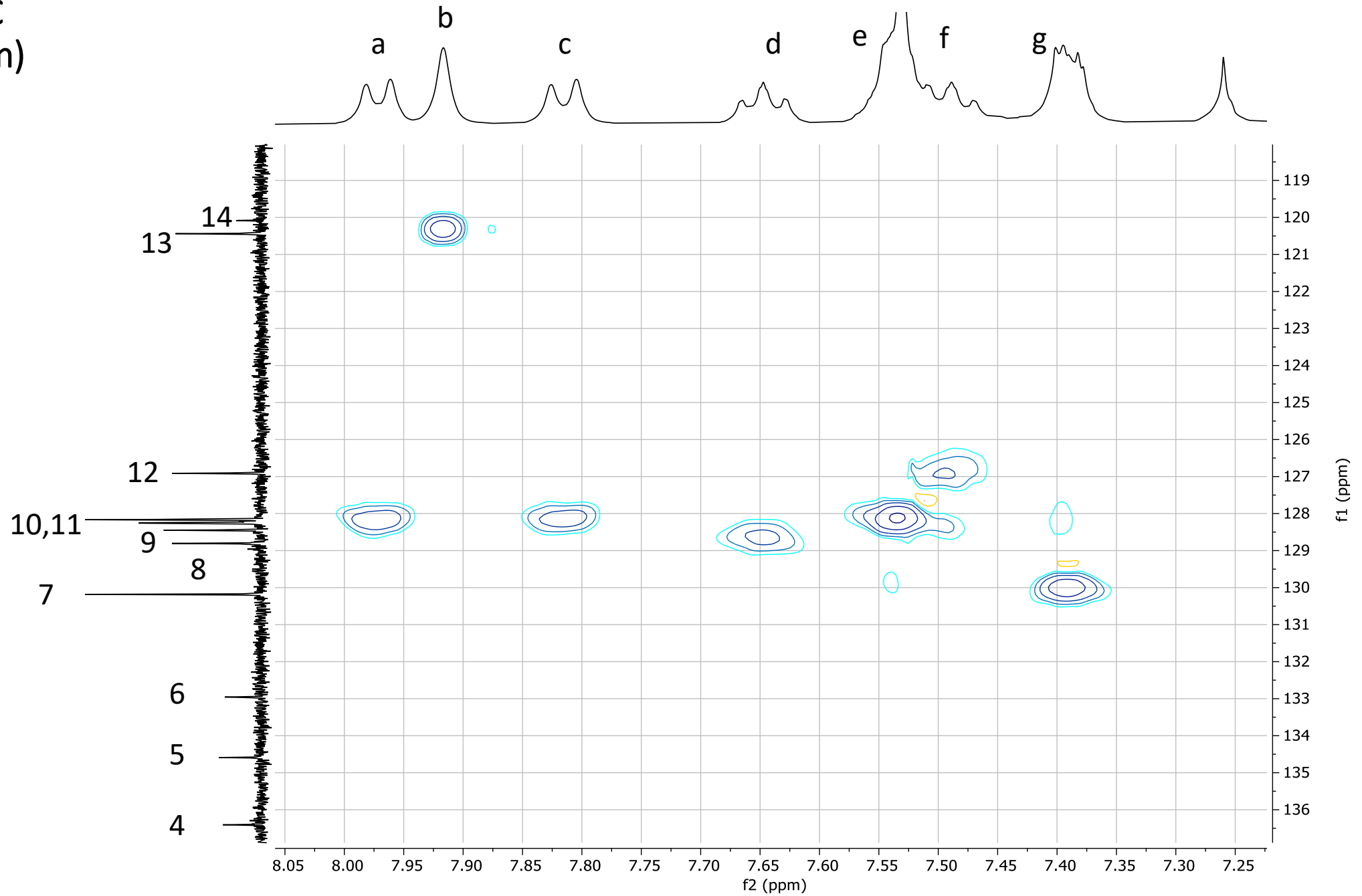
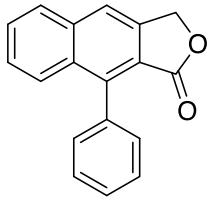


# Type 2 – HSQC Spectrum

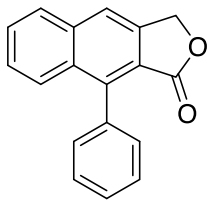




# Type 2 – HSQC Spectrum (Zoom)



# Type 2 – HMBC Spectrum



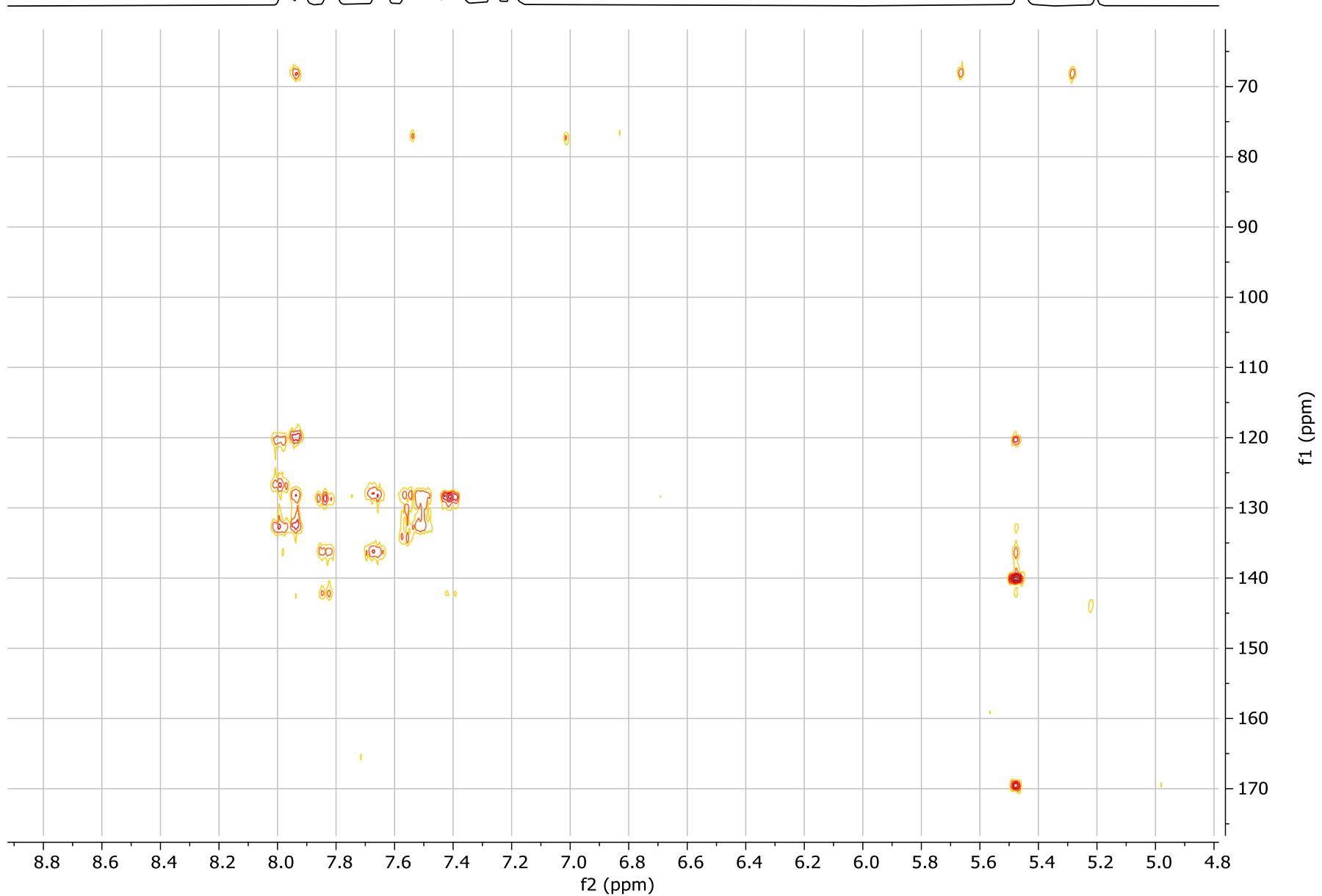
8,9,10,11,12  
7

16

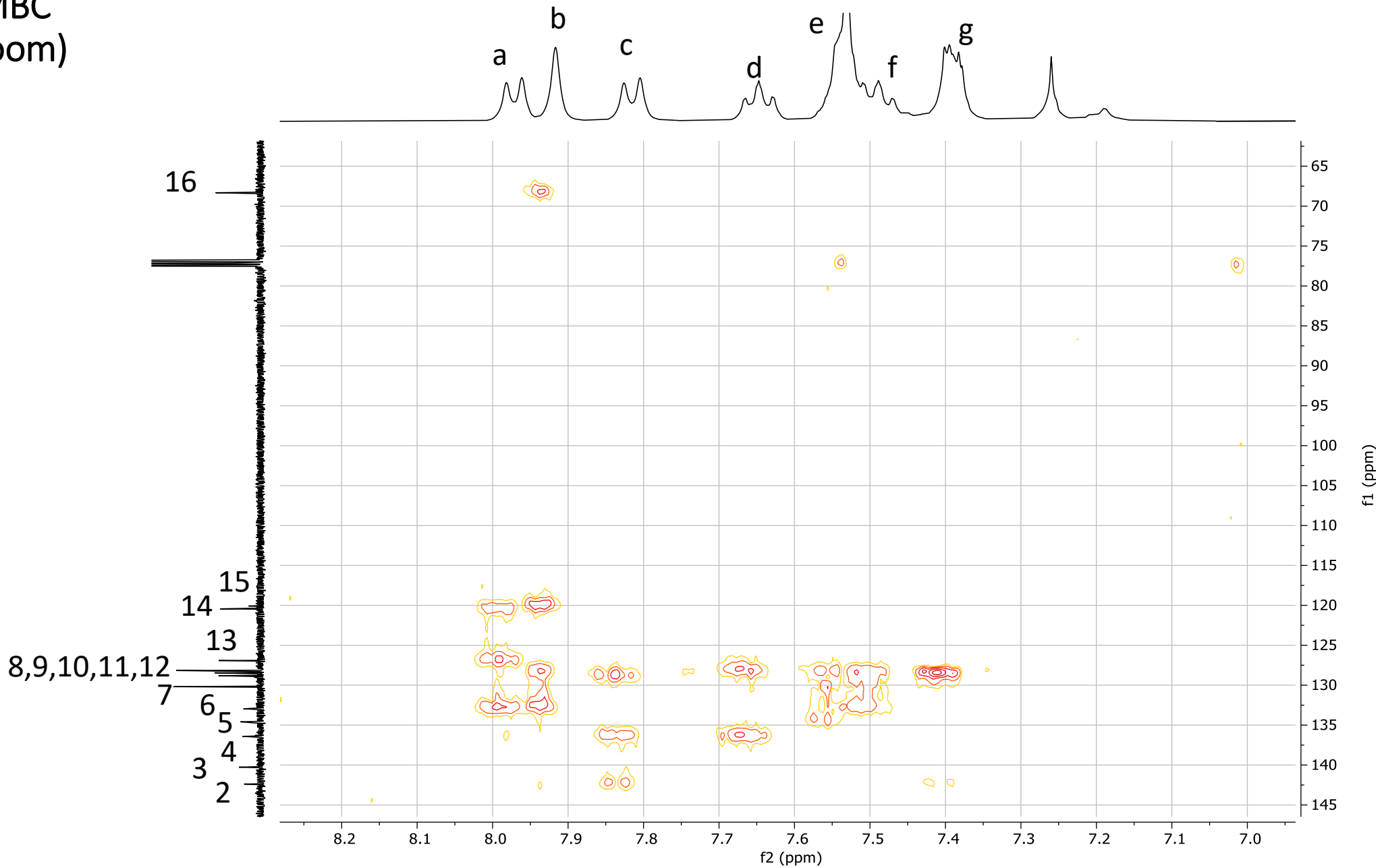
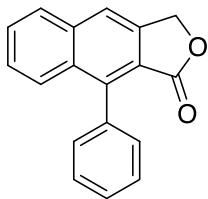
15  
14  
13  
6  
5  
4  
3  
2

1

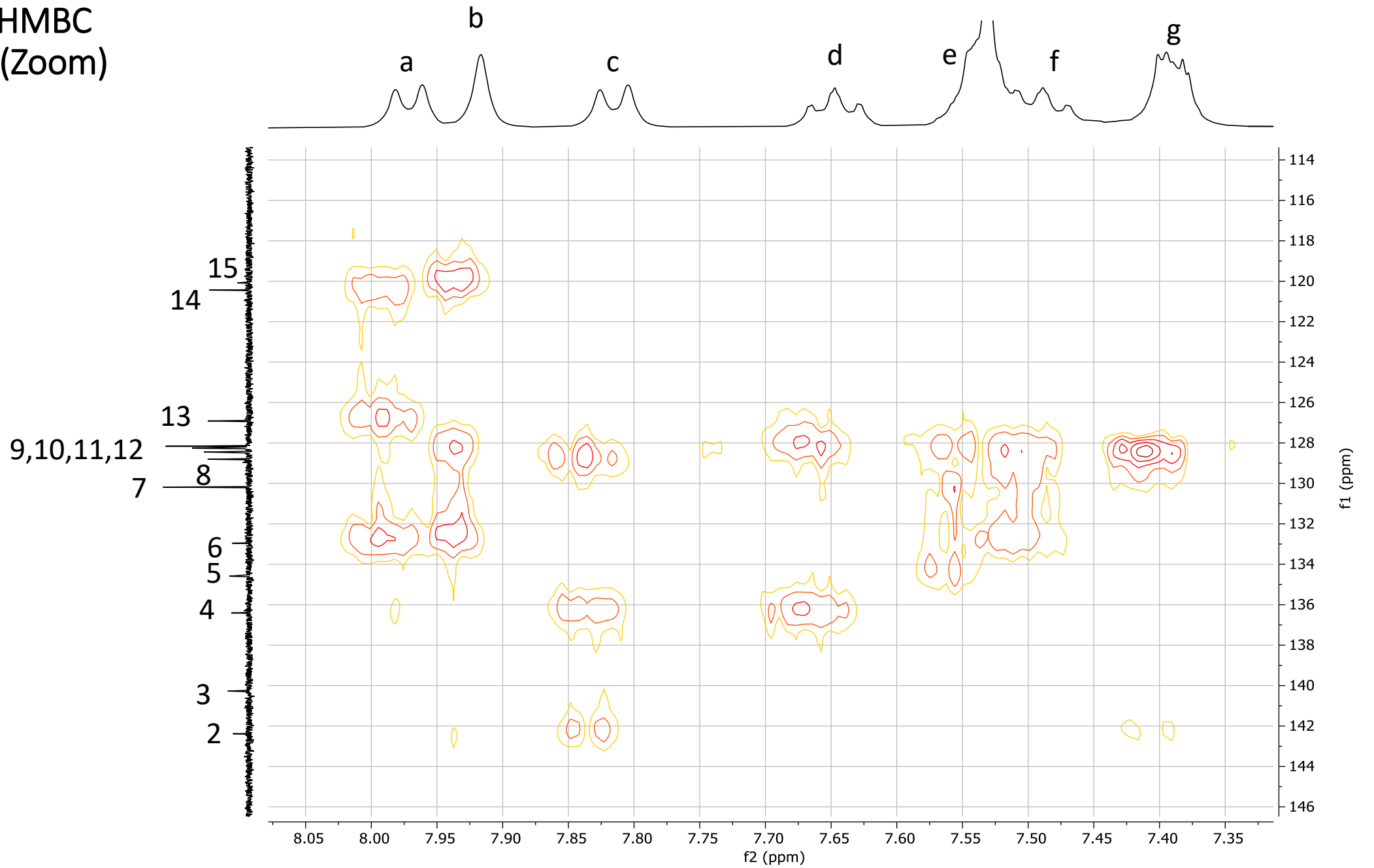
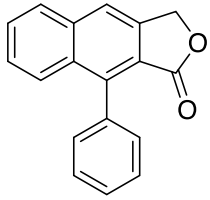
a b c d e f g h



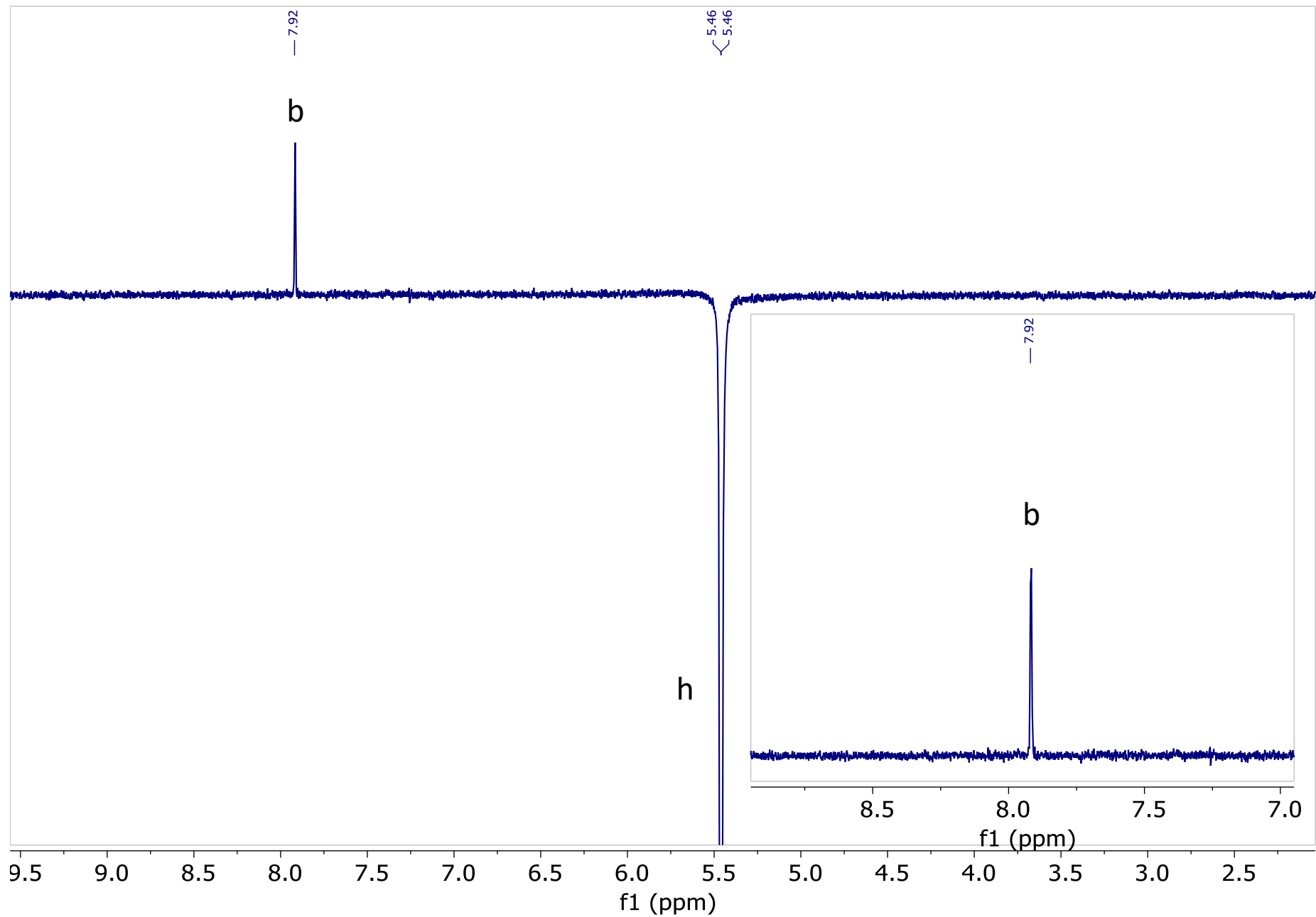
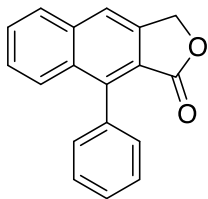
# Type 2 – HMBC Spectrum (Zoom)



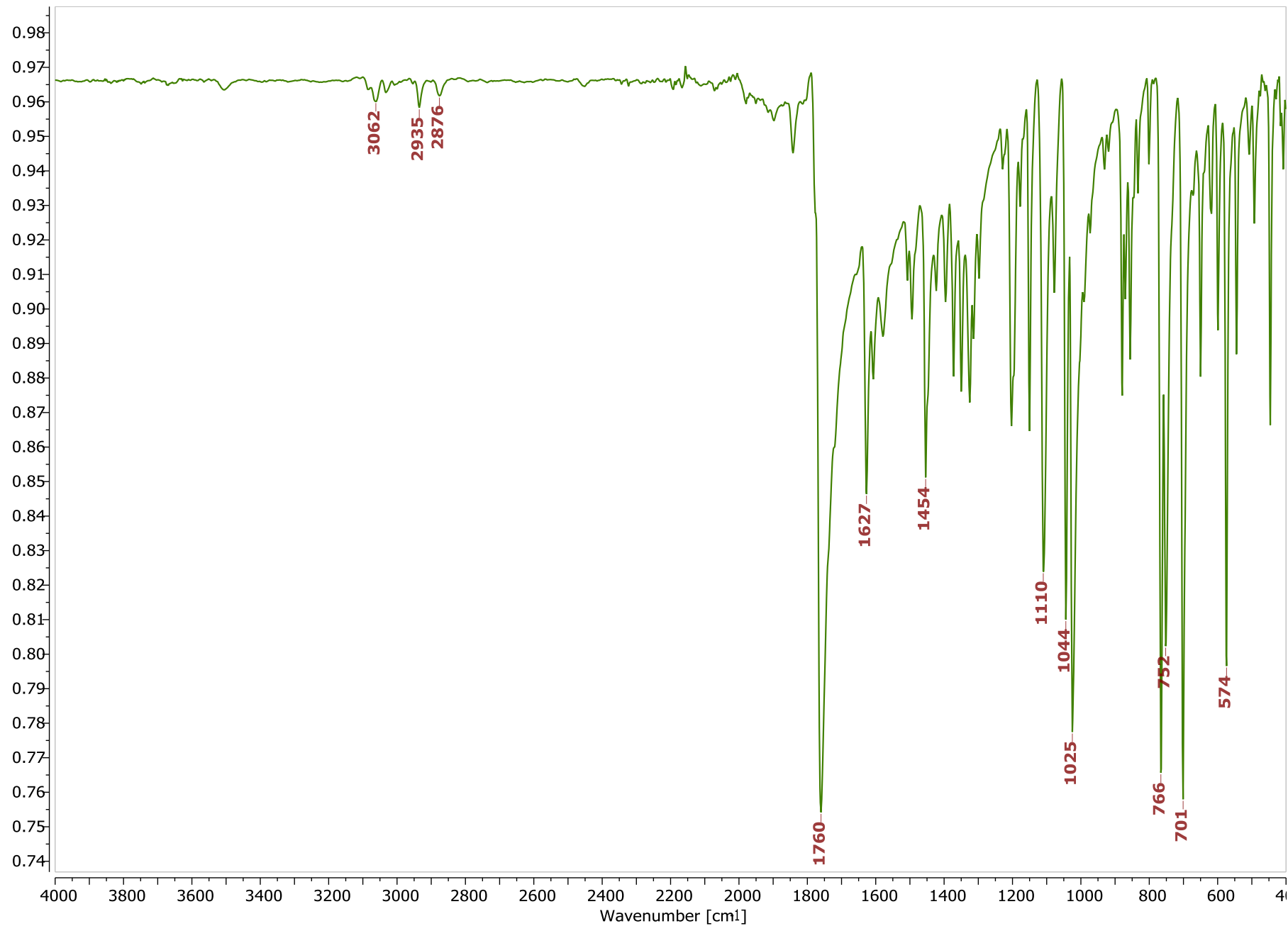
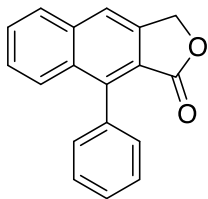
# Type 2 – HMBC Spectrum (Zoom)



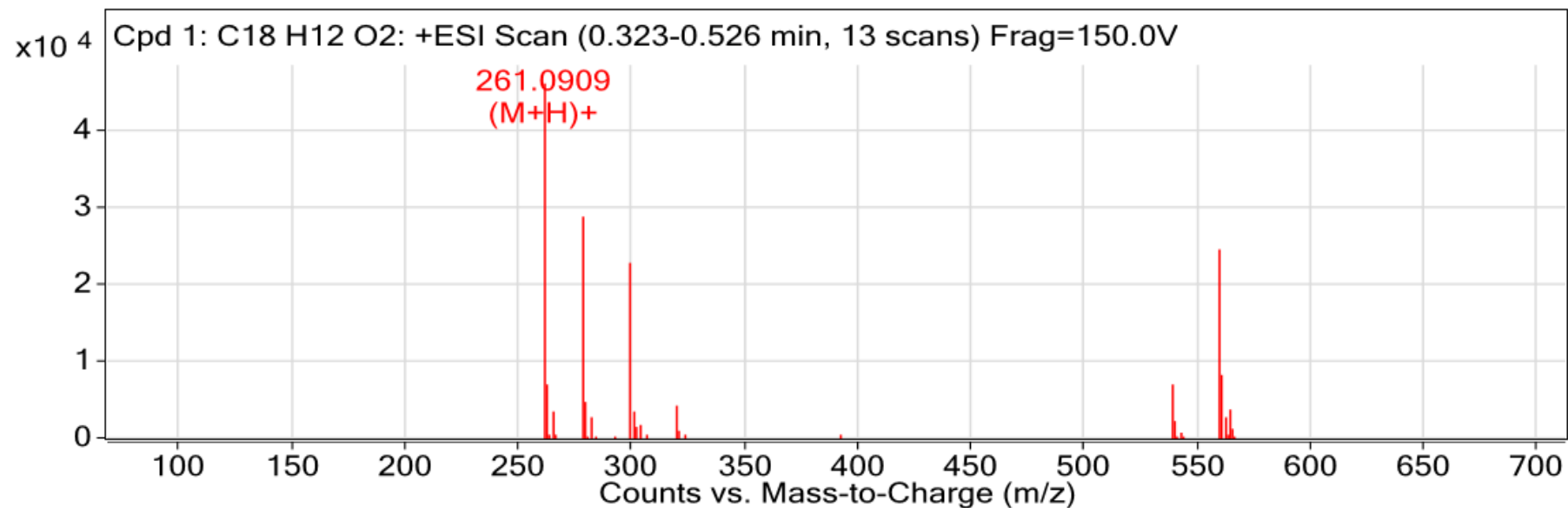
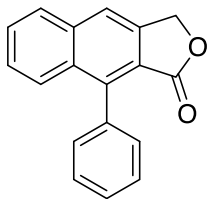
# Type 2 – 1D NOE Spectrum



# Type 2 – IR Spectrum



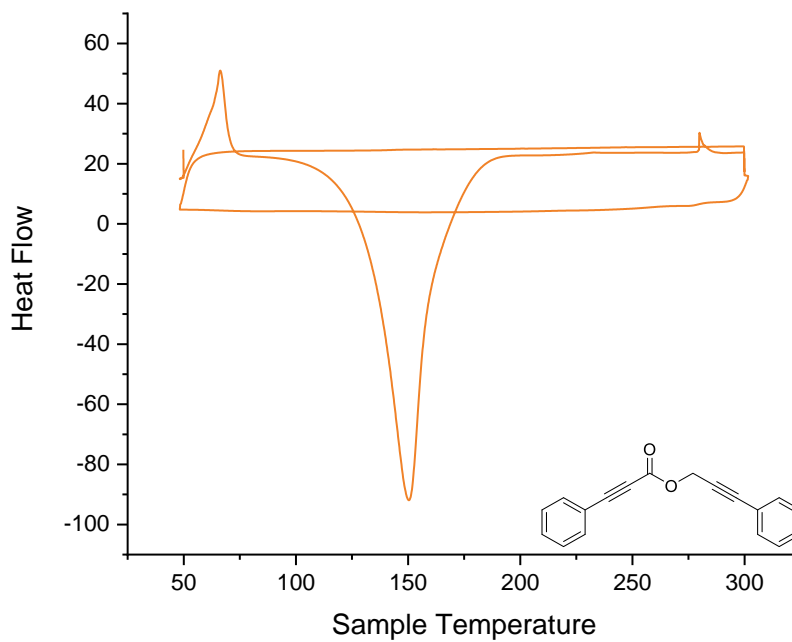
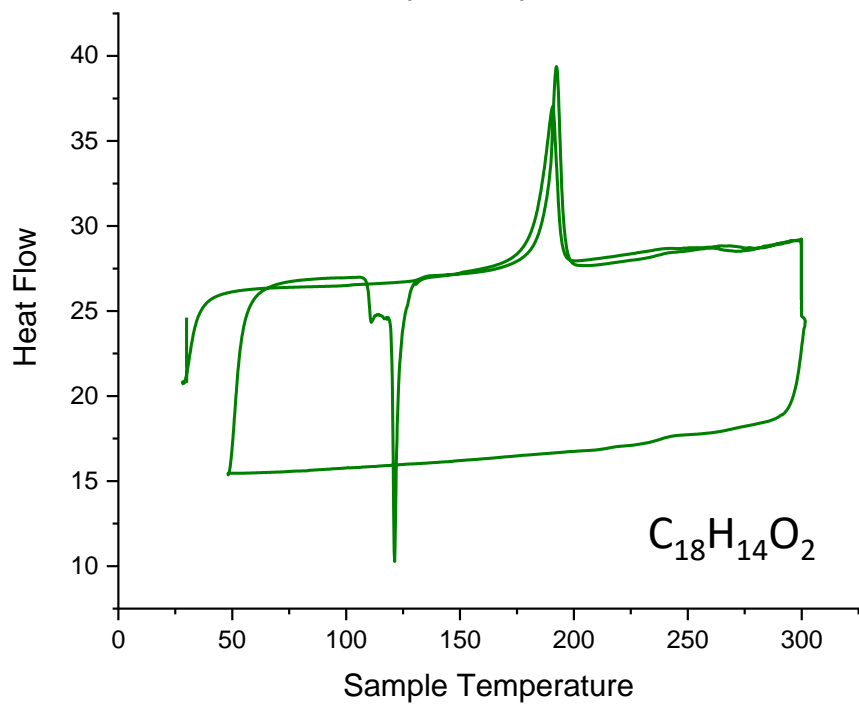
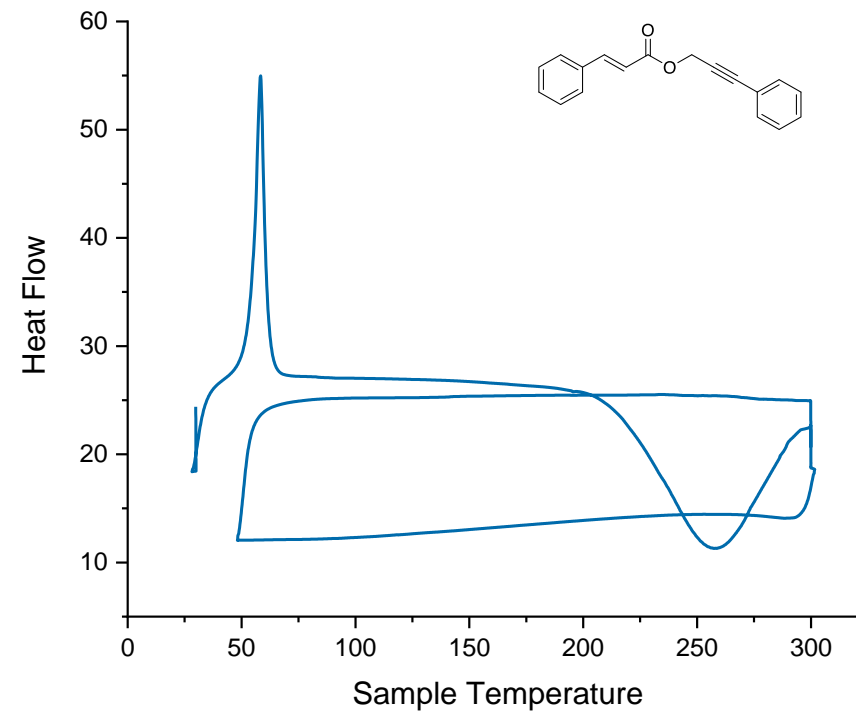
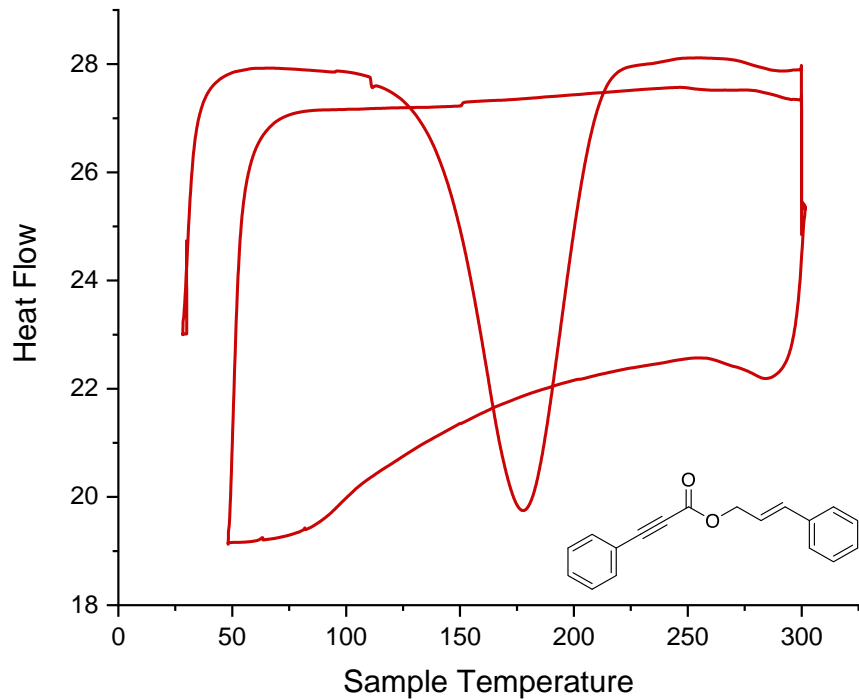
# Type 2 – Mass Spectrum



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
261.0909		46307	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
262.0945		7246	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
263.0974		763	C <sub>18</sub> H <sub>13</sub> O <sub>2</sub>	(M+H) <sup>+</sup>
265.1222		3690		
278.1175	1	29154	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
279.1215	1	5112	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
280.1258	1	479	C <sub>18</sub> H <sub>16</sub> N O <sub>2</sub>	(M+NH <sub>4</sub> ) <sup>+</sup>
299.0472	1	23087	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>
300.0502	1	3665	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>
301.0471	1	1813	C <sub>18</sub> H <sub>12</sub> K O <sub>2</sub>	(M+K) <sup>+</sup>

DSC



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